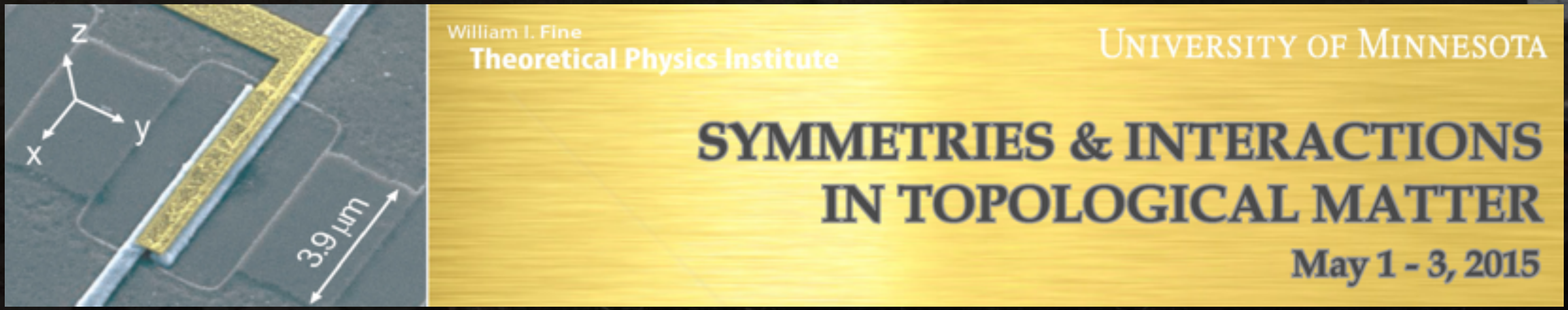
Metal-Insulator Transition and Beyond in the Pyrochlore Iridates

Leon Balents, KITP

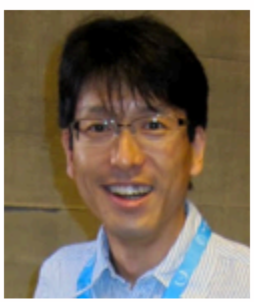


People

Lucile Savary

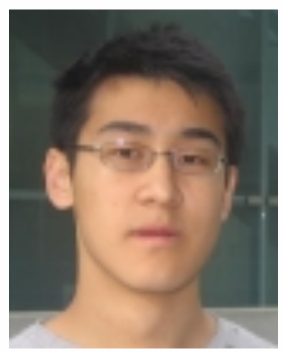
Ru Chen

Eun-Gook Moon



S. Nakatsuji

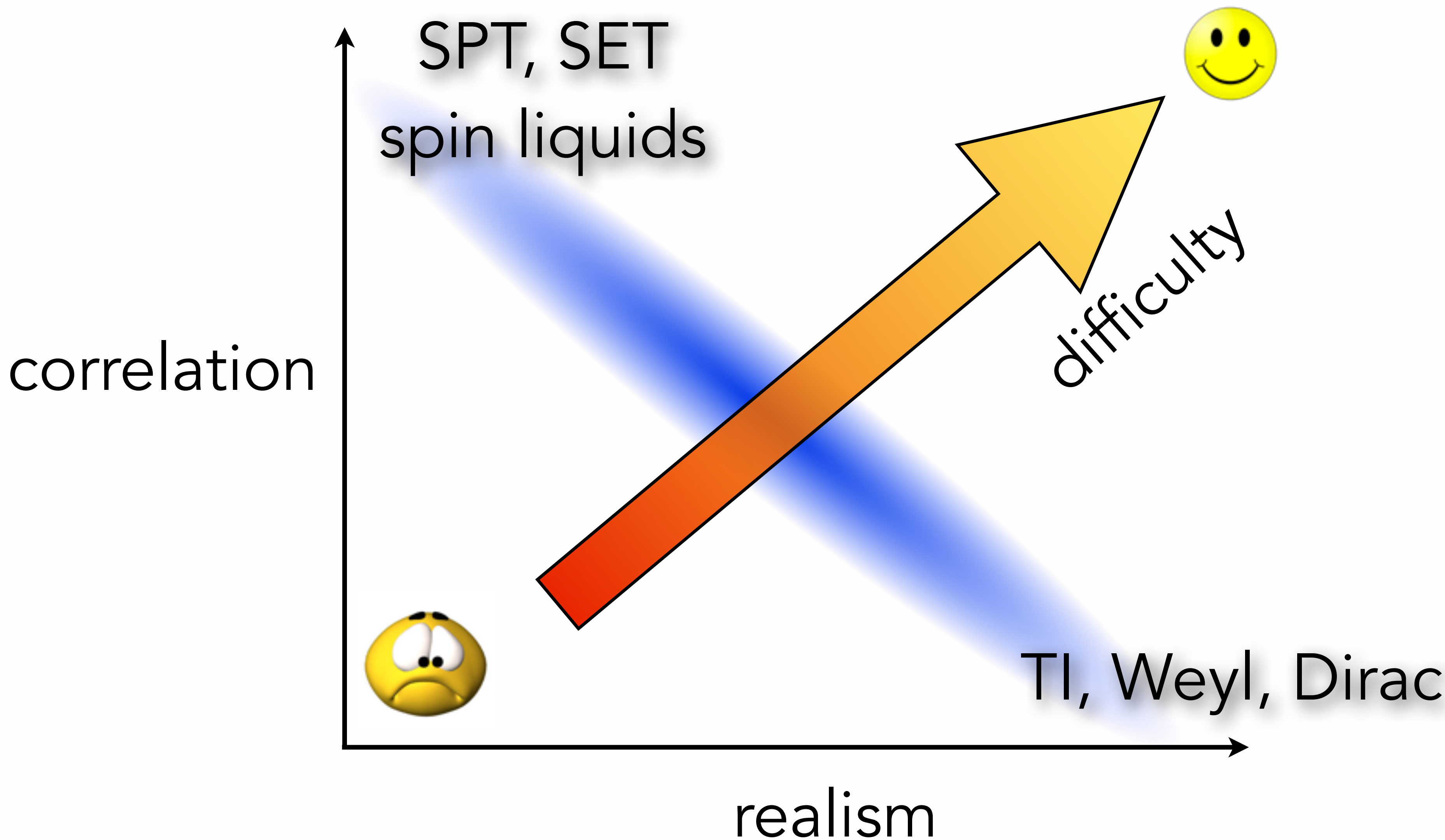
T. Kondo



T. Hsieh

H. Ishizuka

Theory Space



Weyl semimetal

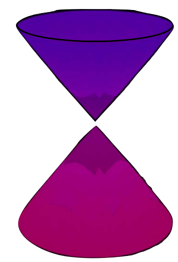
937 PHYSICAL REVIEW

Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING
Princeton University, Princeton, New Jersey
(Received June 16, 1937)

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \rightarrow 0$, for all directions of $\boldsymbol{\kappa}$.

$$H = v\vec{\sigma}\cdot\vec{k}$$



A two-component spinor in three dimensions: “half” of a Dirac fermion. Weyl fermions have a chirality and *must* be massless

Weyl semimetal

937 PHYSICAL REVIEW

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Either inversion or time-reversal (or both) must be broken

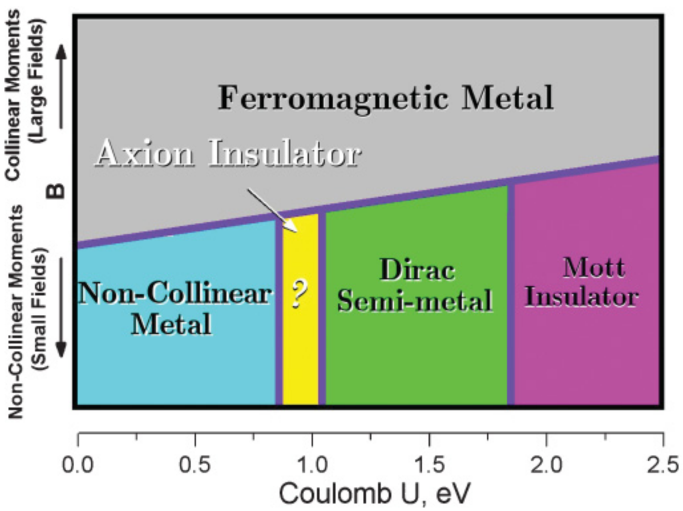
Where it "started"

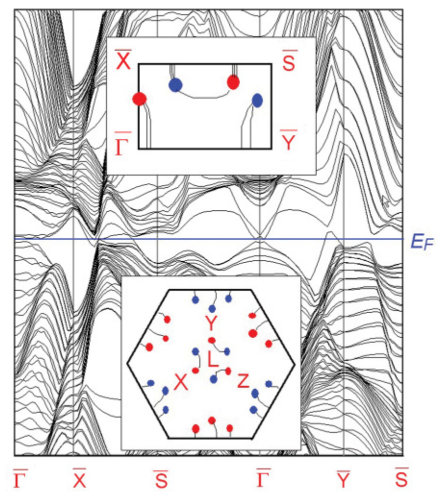
PHYSICAL REVIEW B **83**, 205101 (2011)

Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan,[1] Ari M. Turner,[2] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[1,4]

- Predicted Weyl semimetal in $Y_2Ir_2O_7$ pyrochlore iridate





c.f. Burkov Balents 2011

Where it "started"

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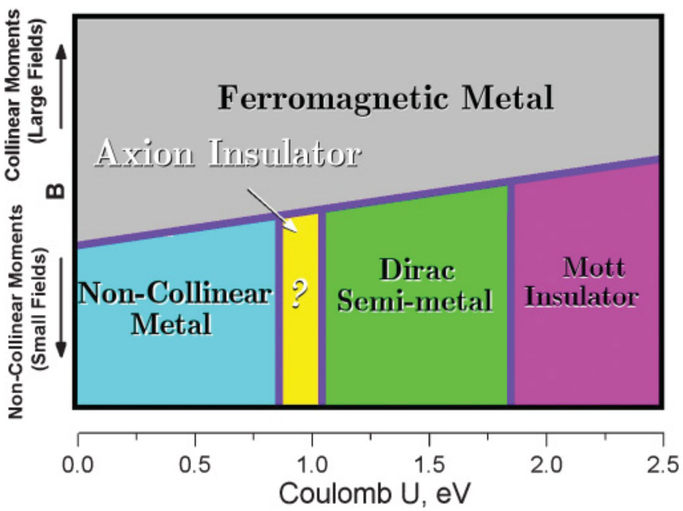
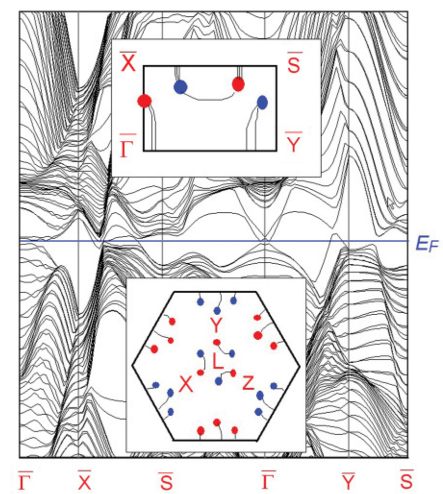
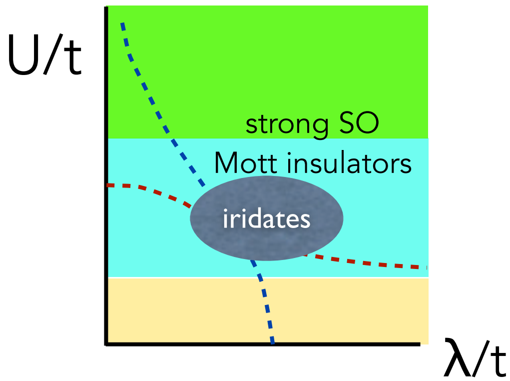




What happened to this thing?

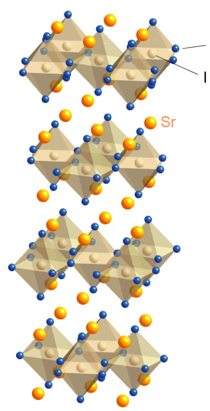
Plan

- Review pyrochlore iridates.
- “Clean” theory
- Less clean reality. Weyl not?

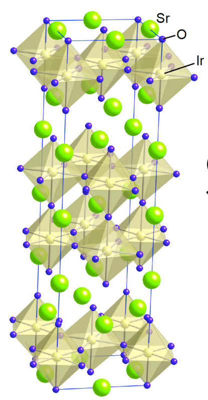


Iridates

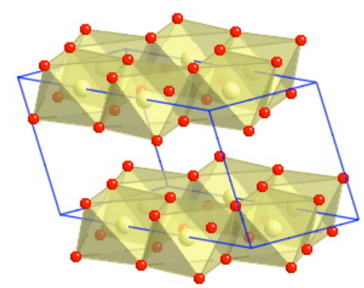
- All energy scales comparable U ~ W ~ λ



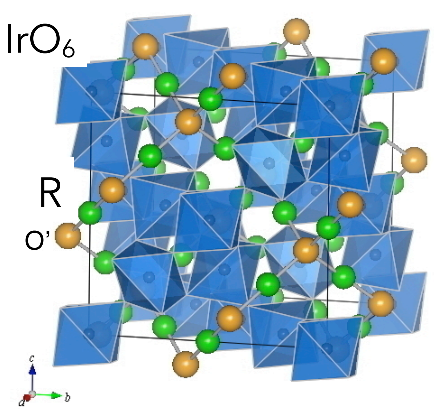
Sr_2IrO_4



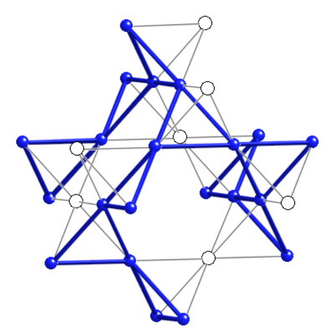
$Sr_3Ir_2O_7$



Na_2IrO_3,
(α,β,γ)-
Li_2IrO_3



$R_2Ir_2O_7$
pyrochlores



$Na_4Ir_3O_8$

Gang Chen + LB, PRB (2008)

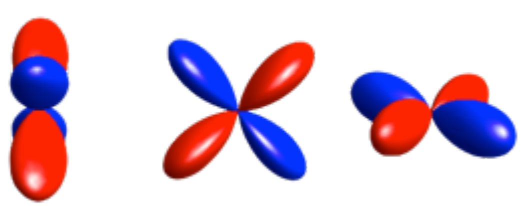
B. J Kim *et al*, Science (2009)

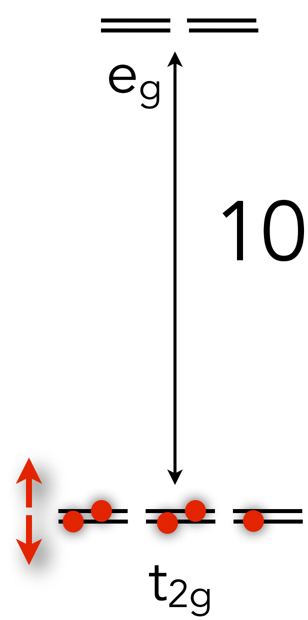
G. Jackeli + G. Khaliullin, PRL (2009)

Spin-Orbit Coupling

Ir^{4+}=5d^5

octahedral coordination





10Dq ~ 2eV

$$P_{t_{2g}}\mathbf{L}P_{t_{2g}} = -\mathsf{L}_{\text{eff}}$$

$$\ell_{\text{eff}} = 1$$

$$H_{SOC} = -\lambda \mathsf{L}_{\text{eff}} \cdot \mathsf{S}$$

Gang Chen + LB, PRB (2008)

B. J Kim *et al*, Science (2009)

G. Jackeli + G. Khaliullin, PRL (2009)

Spin-Orbit Coupling

$Ir^{4+} = 5d^5$

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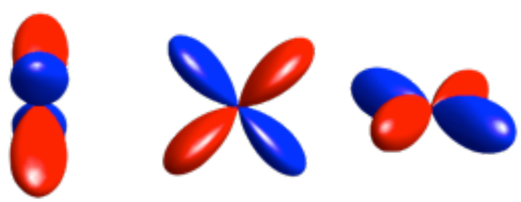
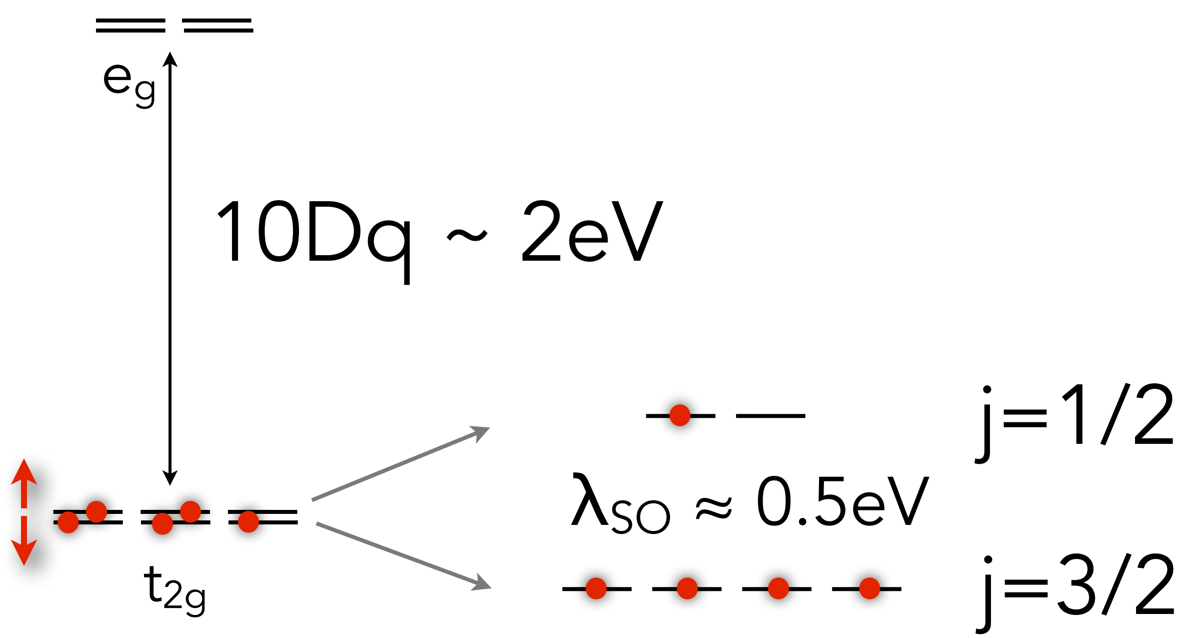
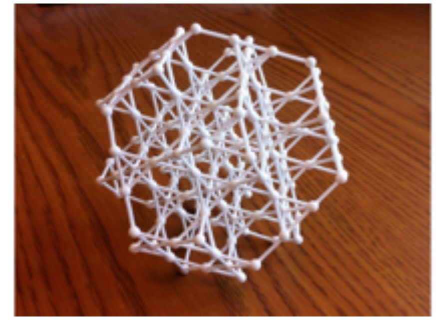


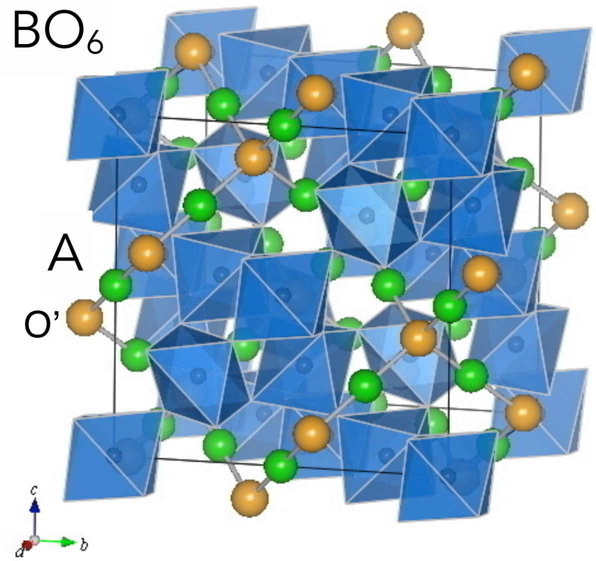


Note: only Kramer's degeneracy remains. SOC tends to suppress Jahn-Teller effects.

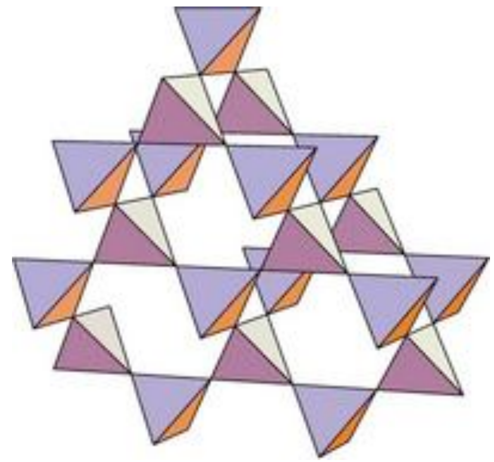
Pyrochlores



http://www.shapeways.com/shops/cmm.html



$A_2B_2O_7$



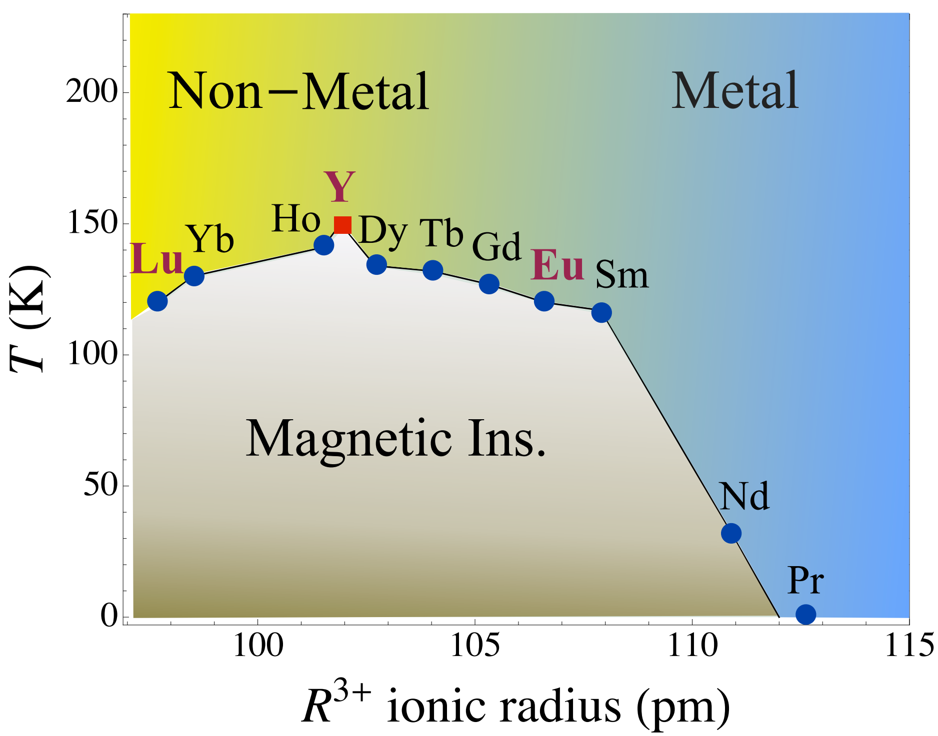
A (B) sublattice

A=Y,Ln ⟵ f-electron moments, except when A = Y, Eu

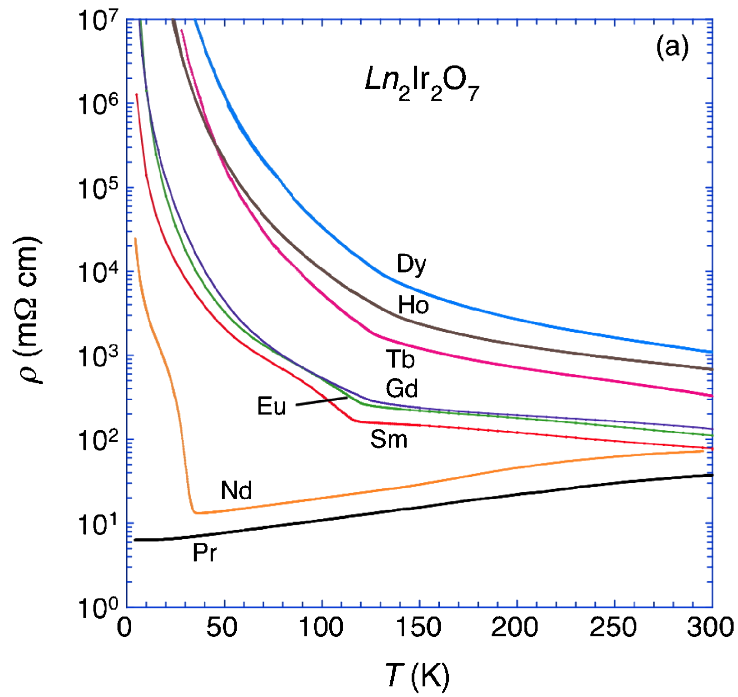
B = Ir

Pyrochlore iridates

- Continuous magnetic/metal-insulator transitions

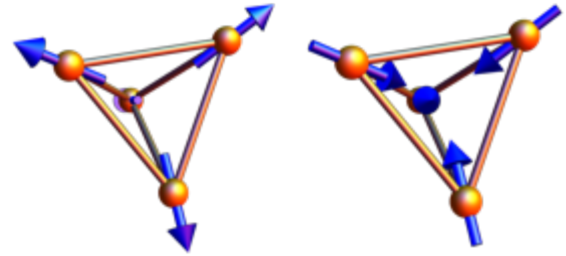


Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

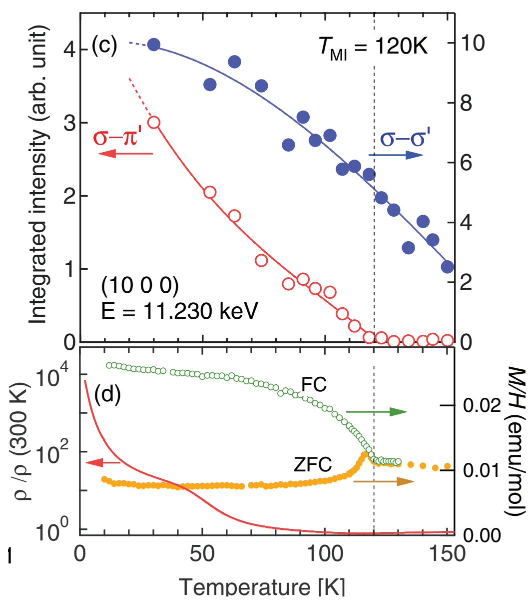


K. Matsuhira et al, JPSJ 2011

AIAO order

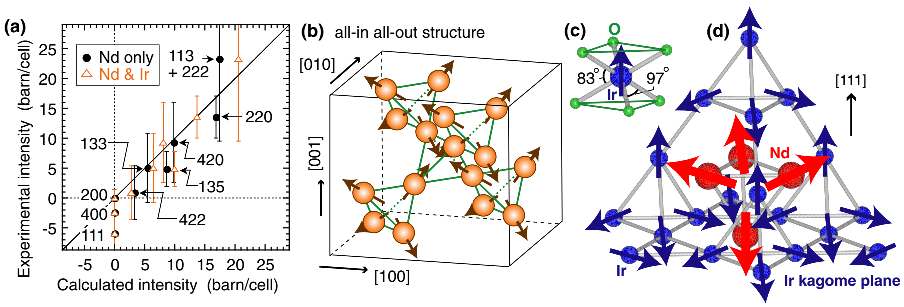


- Growing evidence in many materials



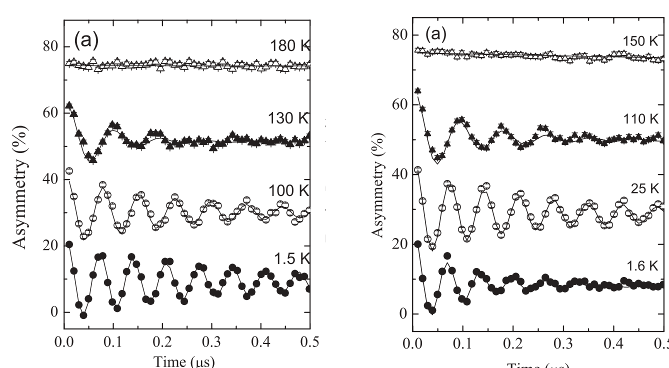
$Eu_2Ir_2O_7$

H. Sagayama *et al*, 2013



$Nd_2Ir_2O_7$

K. Tomiyasu *et al*, 2012



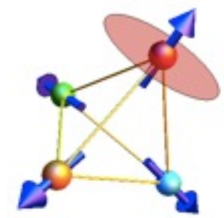
$Y_2Ir_2O_7$, $Yb_2Ir_2O_7$

S. Disseler *et al*, 2012

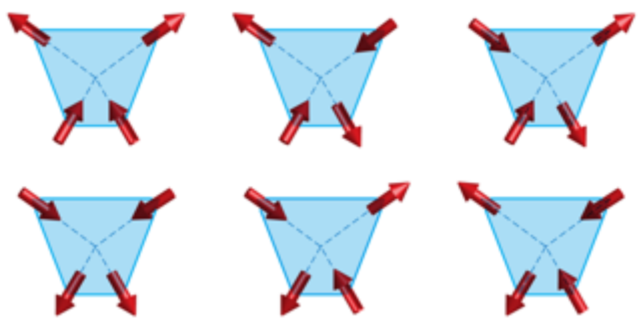
Local moment picture

- Ising model

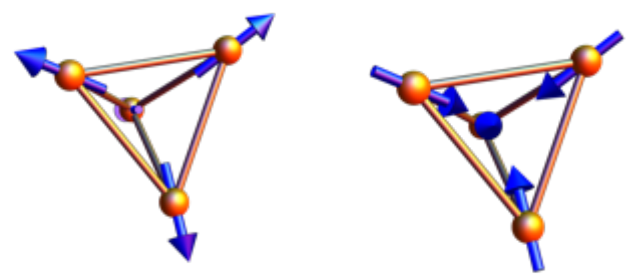
$$H = J_z \sum_{\langle i,j \rangle} S_i^z S_j^z$$



local z axes



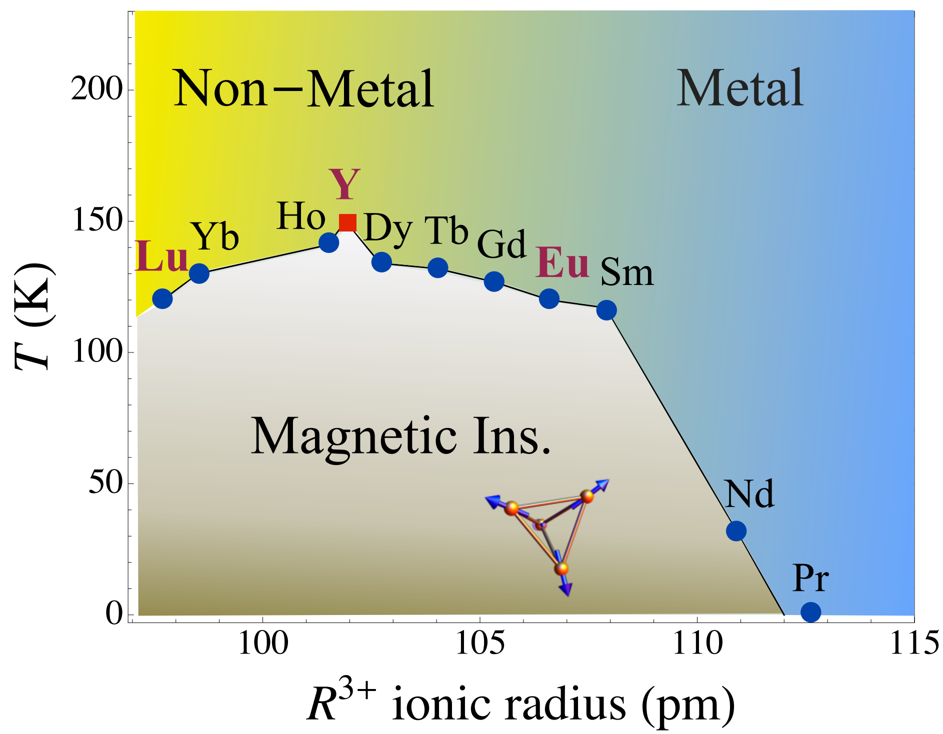
$J_z > 0$: spin ice



$J_z < 0$: all-in/all-out order

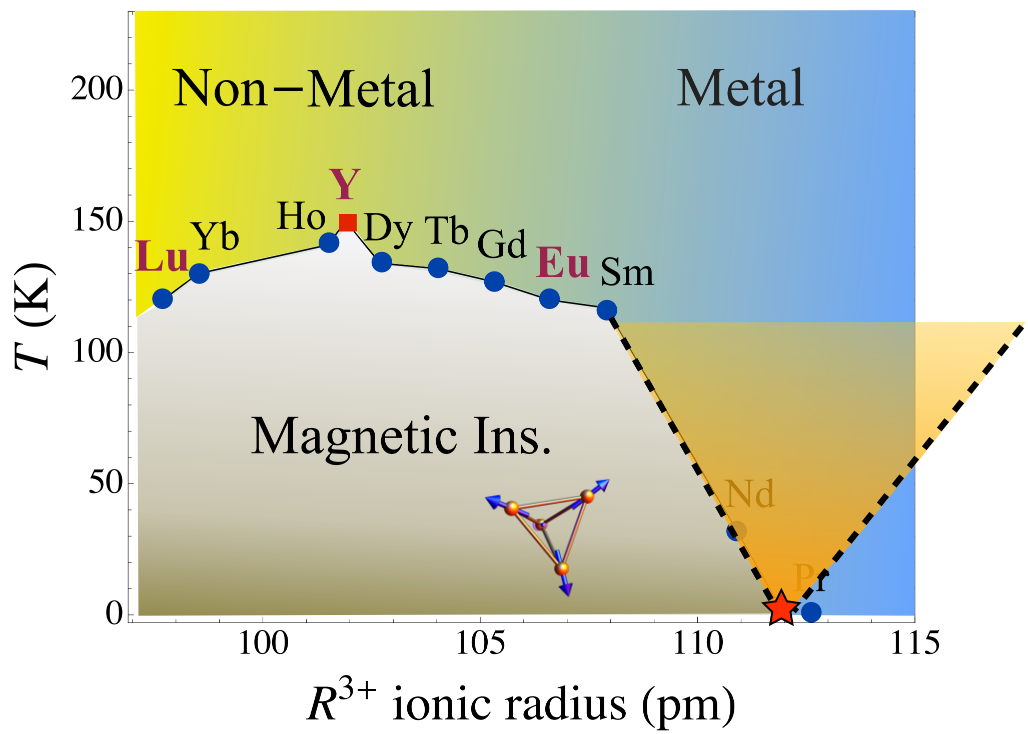
Quantum criticality

How does magnetic order onset?



Quantum criticality

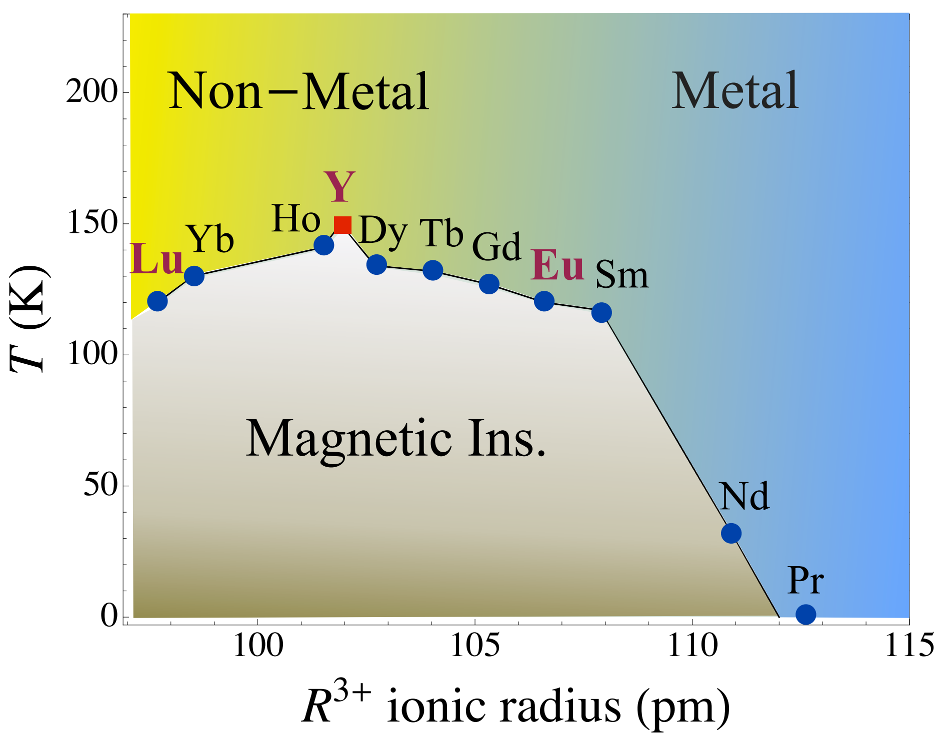
How does magnetic order onset?



QCP?

Pyrochlore iridates

- Continuous magnetic/metal-insulator transitions

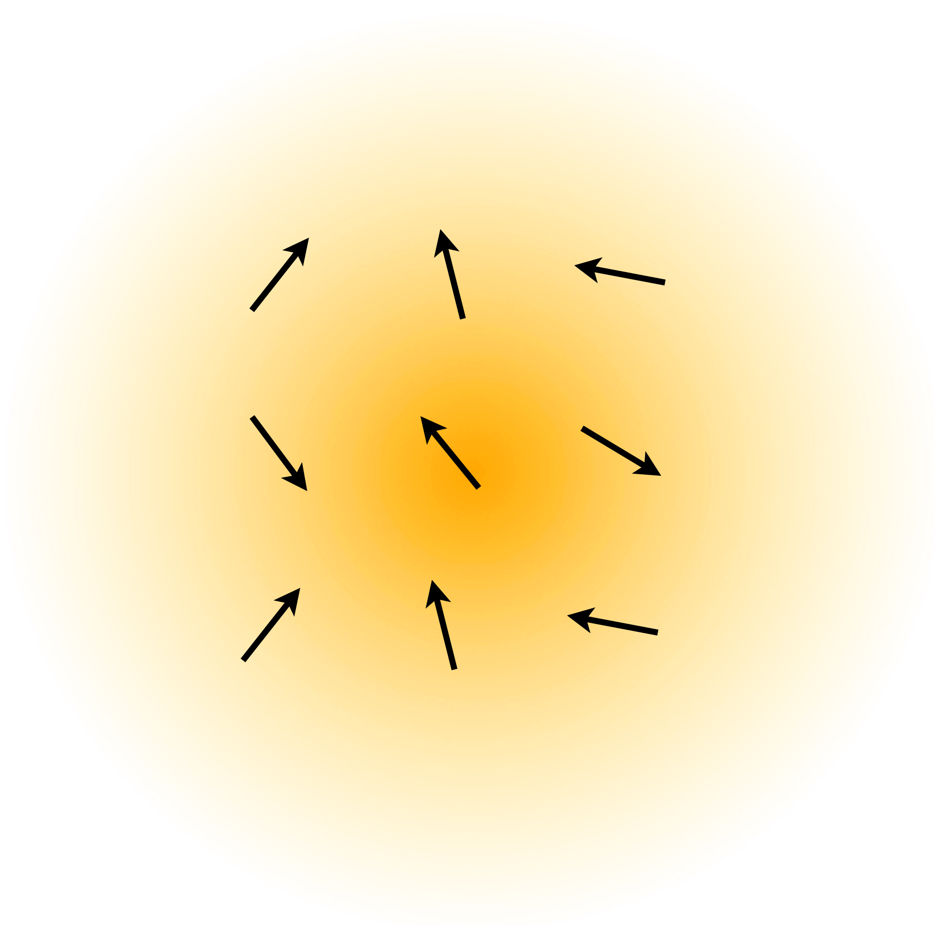


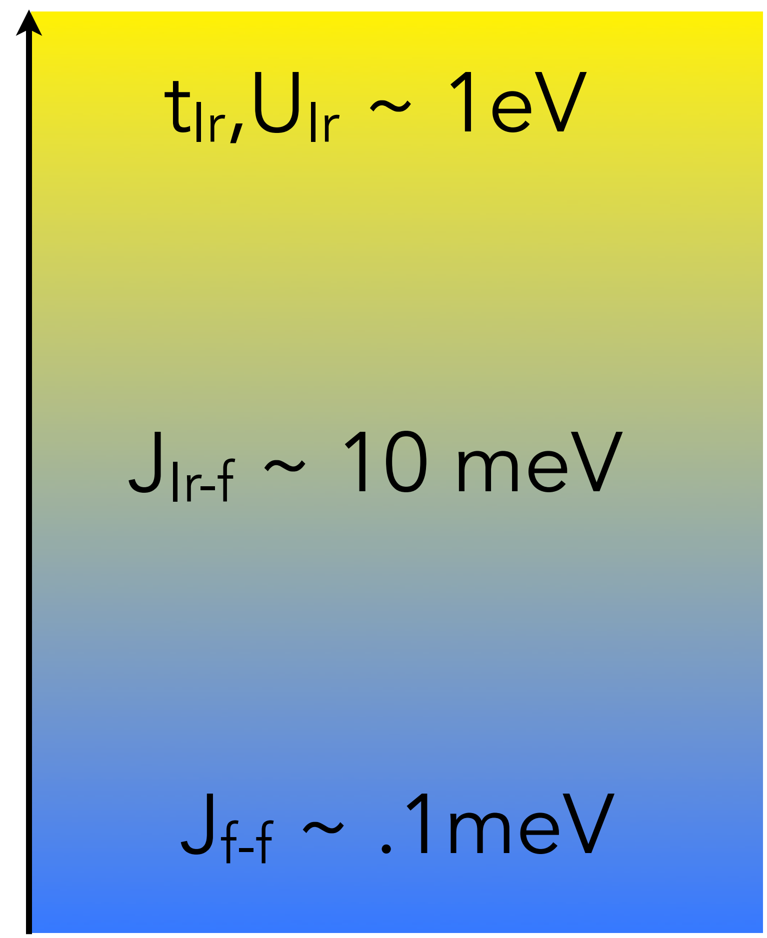
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

note: Y, Eu fit on the same plot. Indicates f electron spins play a secondary role

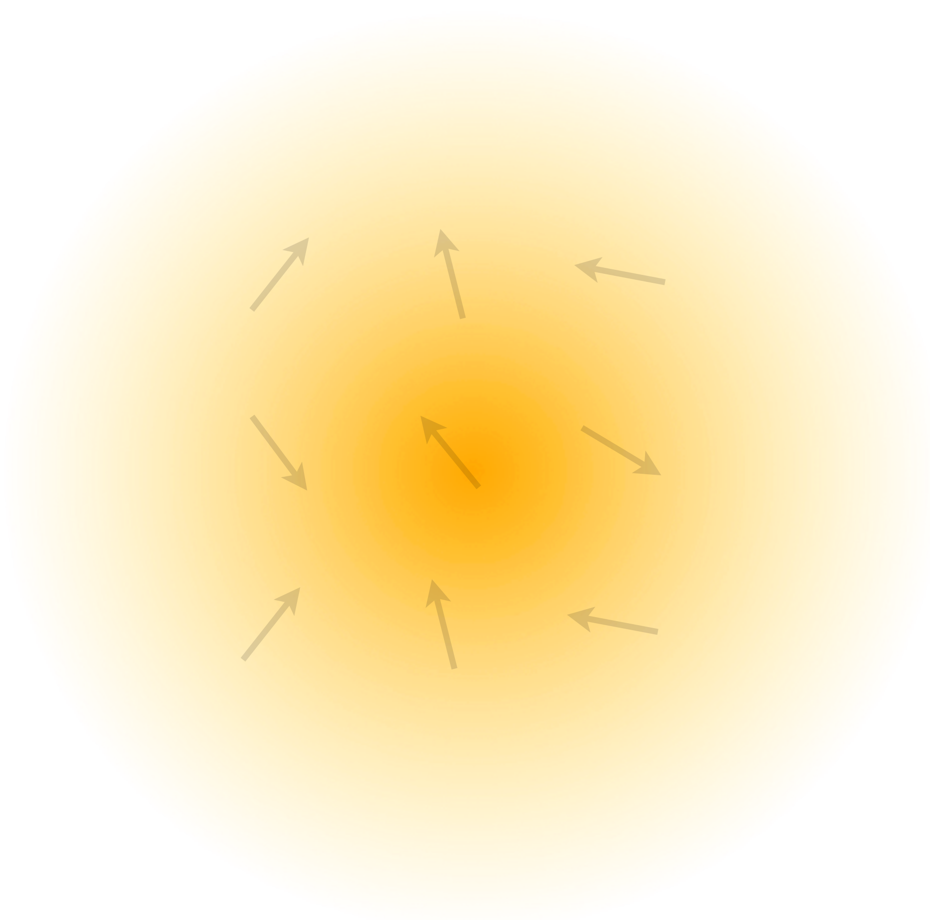
c.f. $J_{\text{spin ice}} \sim 1\text{K}$

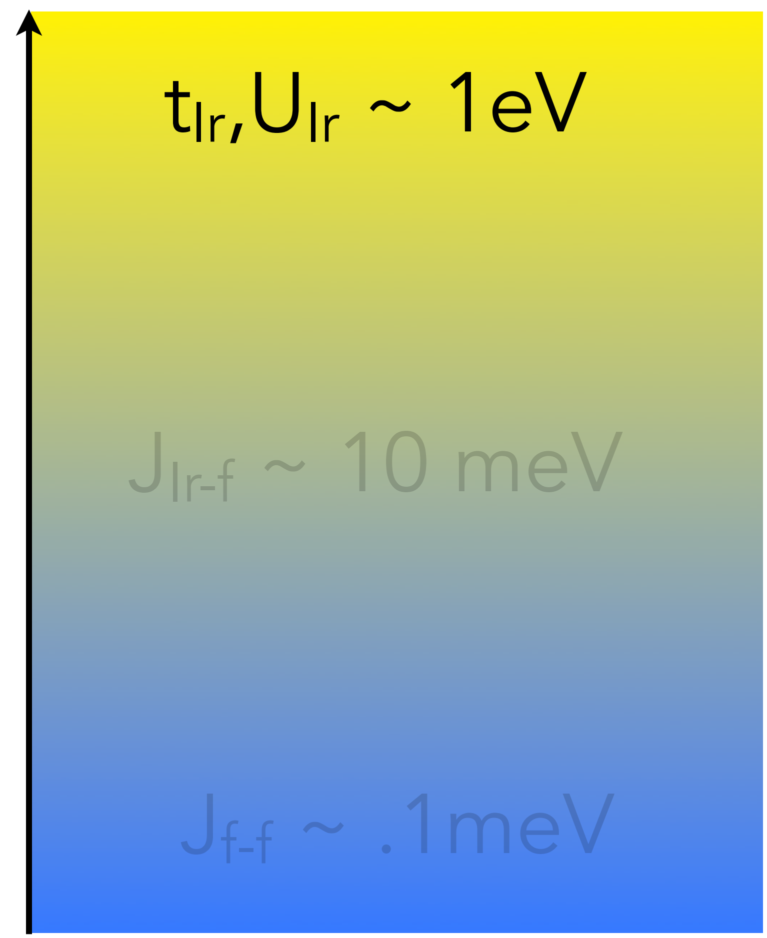
Energy scales





Energy scales

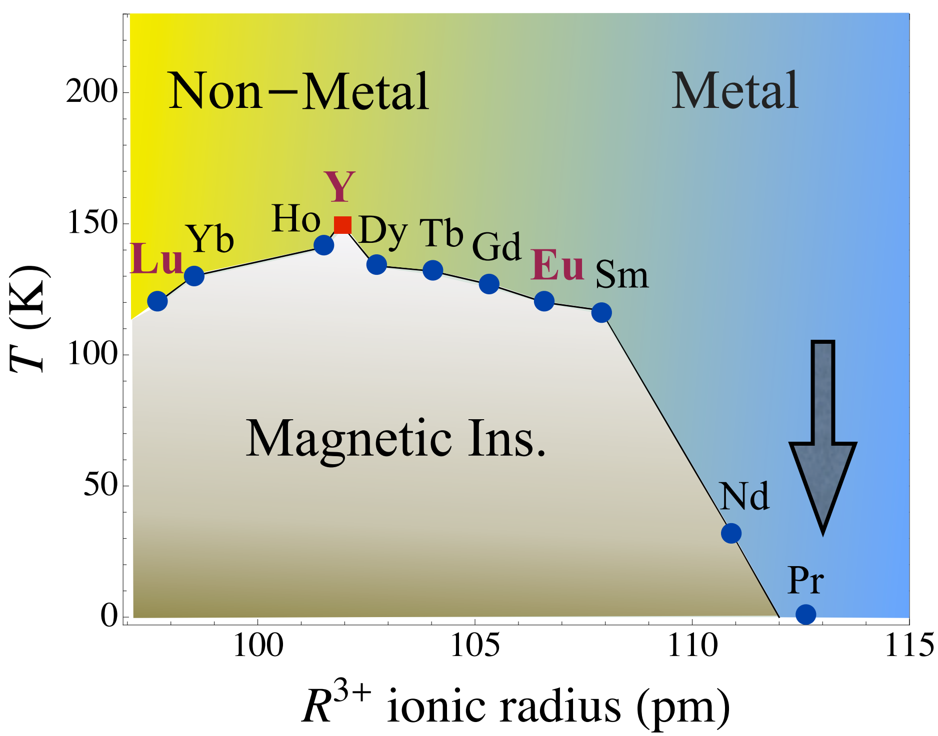




Neglect rare earths at first cut

Pyrochlore iridates

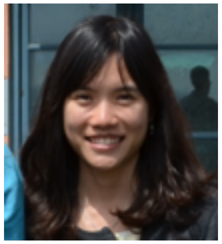
- Itinerancy?



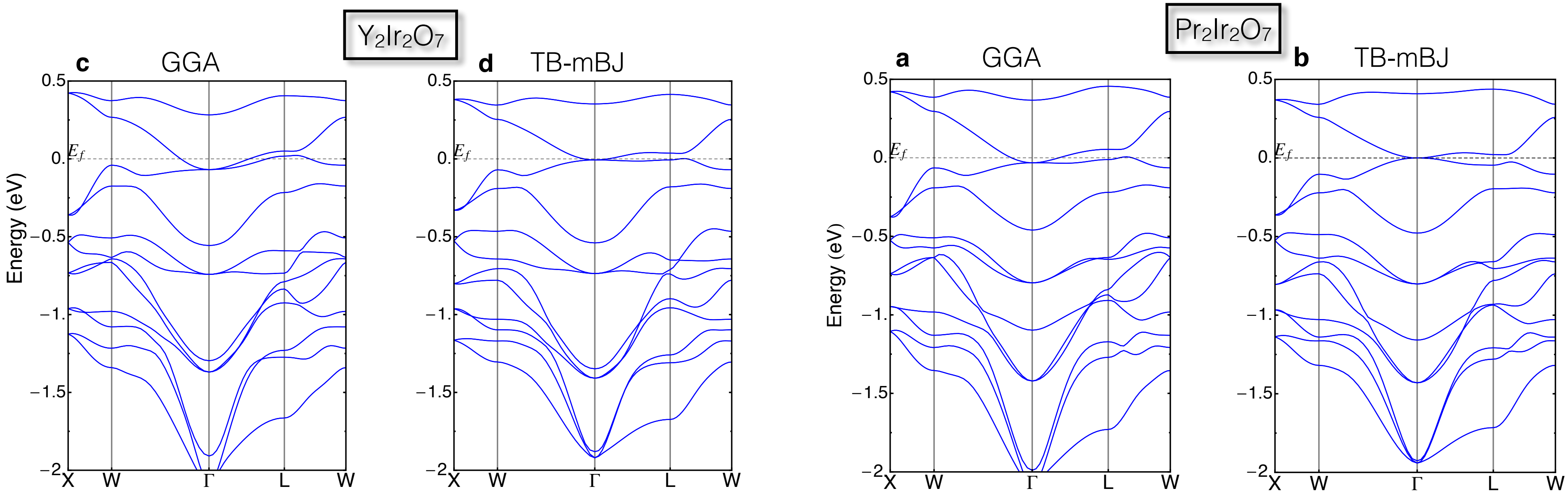
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

what is the “parent” paramagnetic structure?

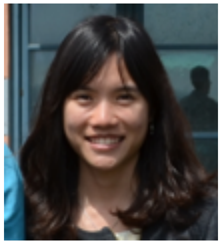
paramagnetic, GGA+SO, Wien2k



Electronic structure

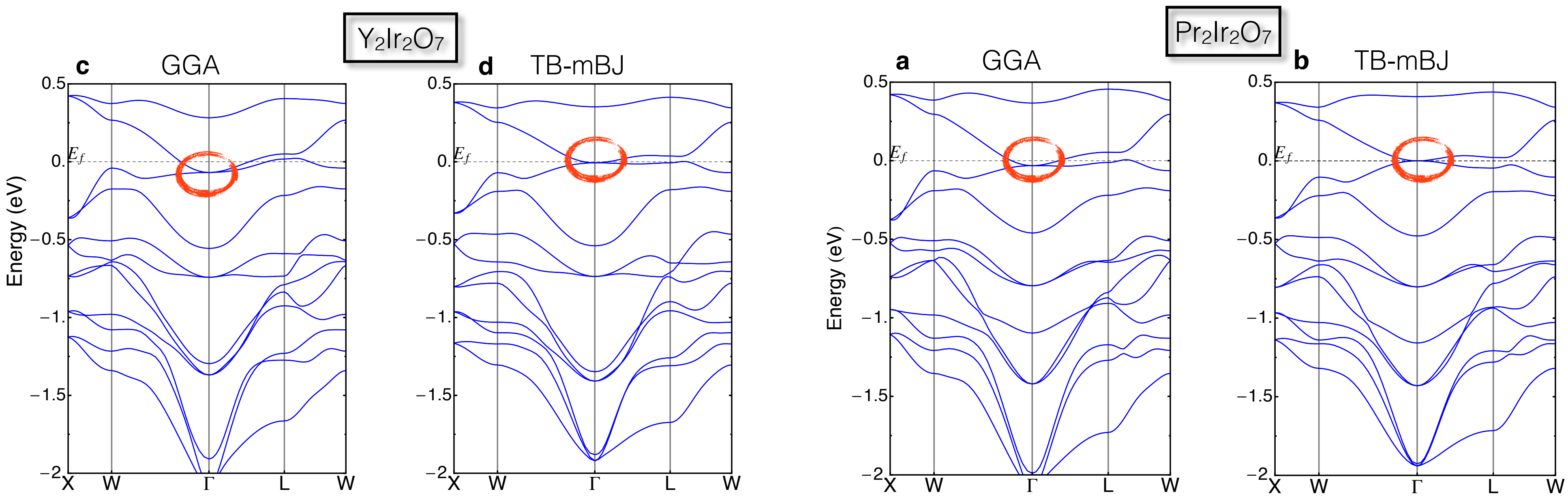


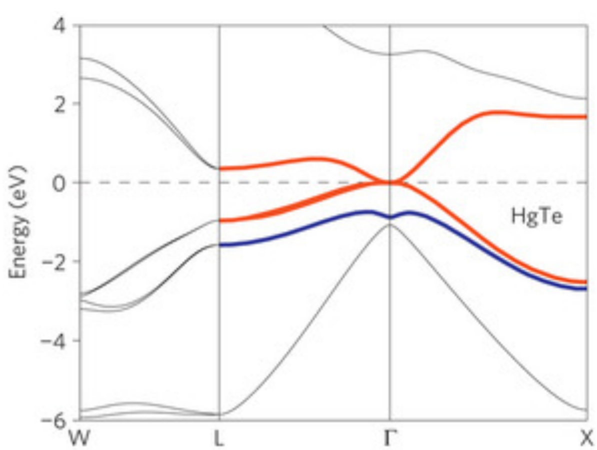
primarily Ir 5d bands



paramagnetic, GGA+SO, Wien2k

Electronic structure



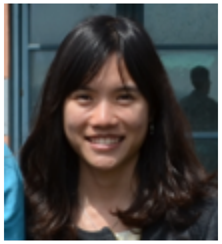


Γ_8 4-dimensional irrep

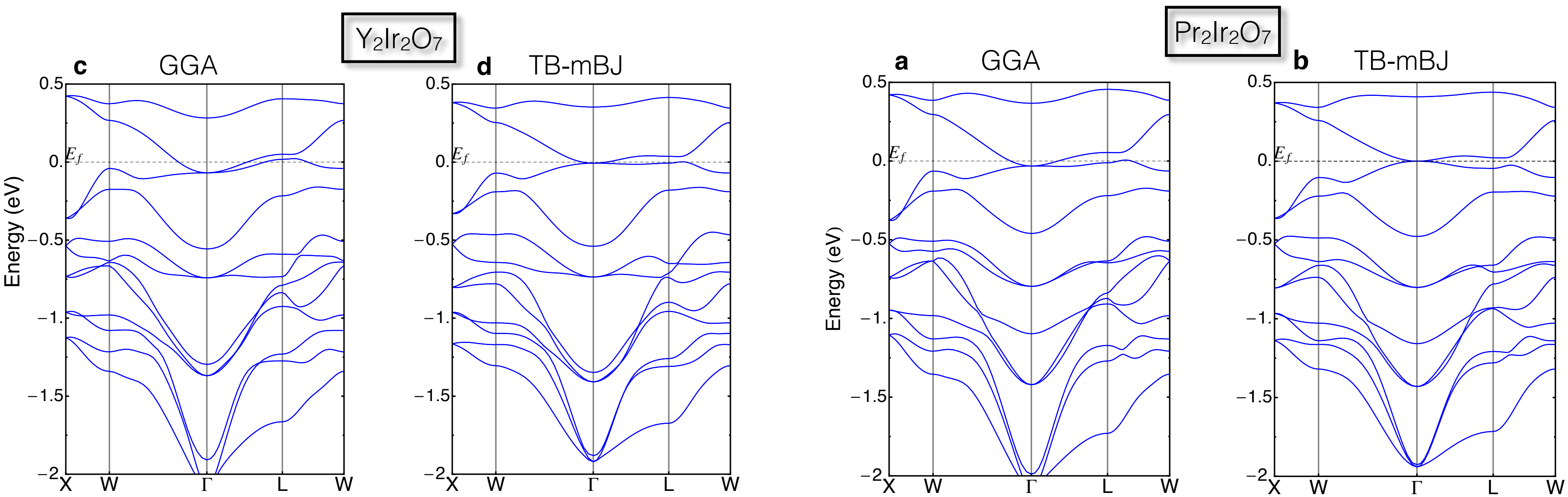
guaranteed by cubic symmetry

and time reversal

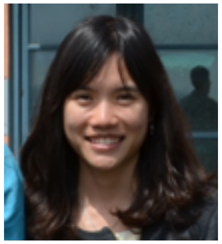
paramagnetic, GGA+SO, Wien2k



Electronic structure

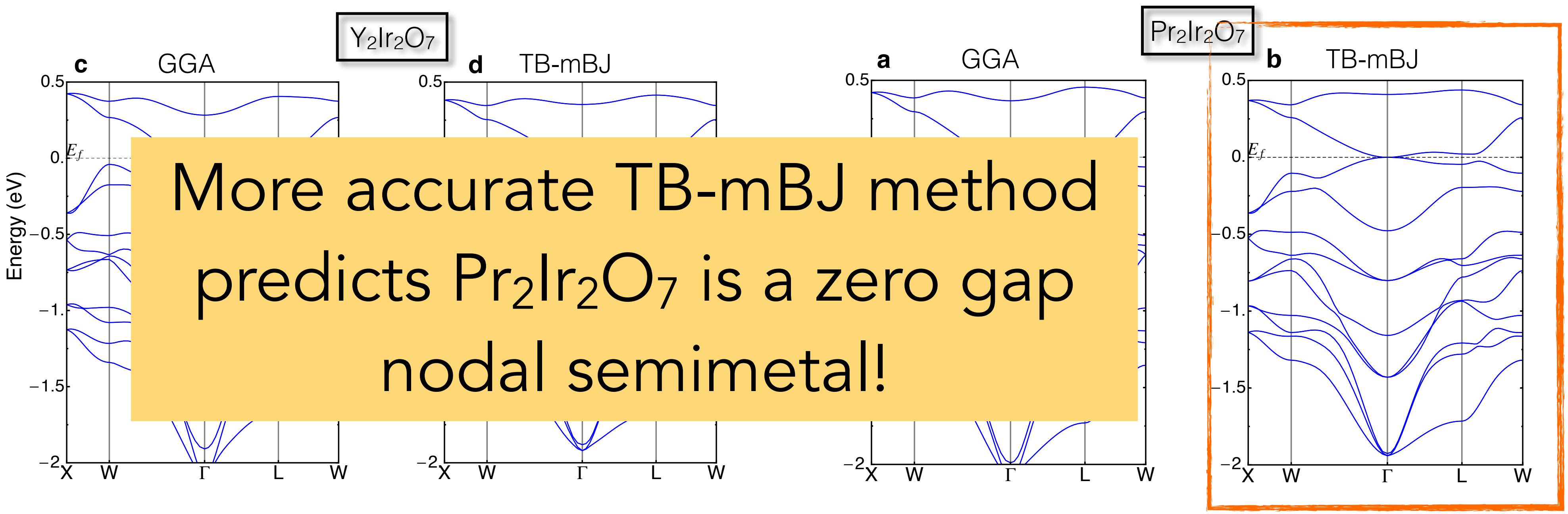


Band bending decreases with increasing rare earth radius



paramagnetic, GGA+SO, Wien2k

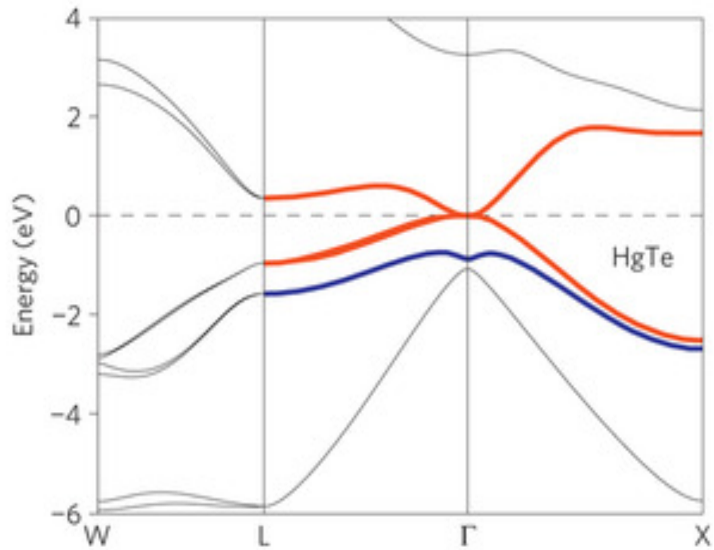
Electronic structure



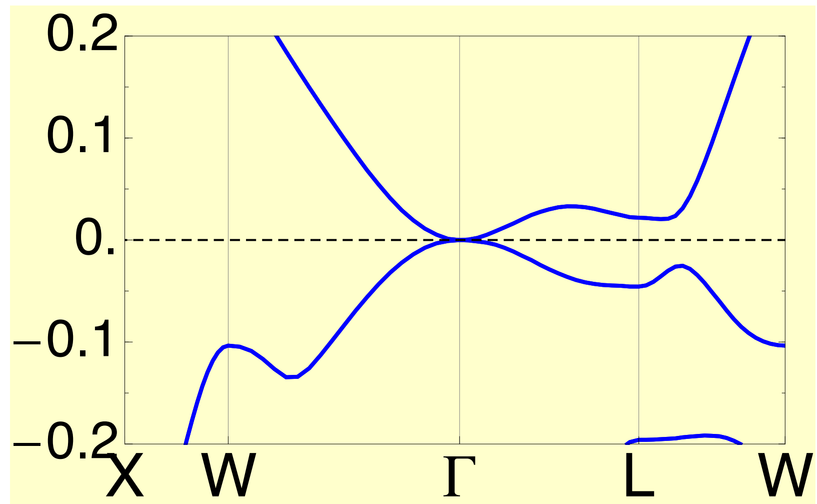
More accurate TB-mBJ method predicts $Pr_2Ir_2O_7$ is a zero gap nodal semimetal!

Band bending decreases with increasing rare earth radius

Quadratic band touching



HgTe



$Pr_2Ir_2O_7$

Mathematically identical band touching! But <u>note energy scales</u>

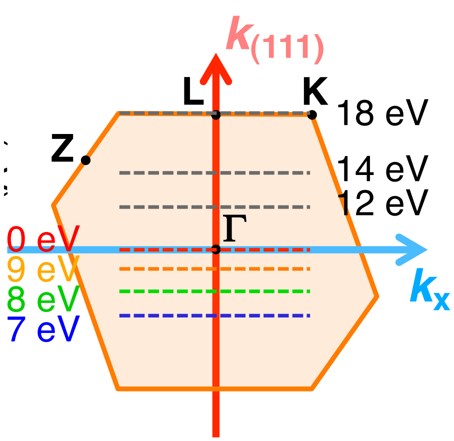
ARPES

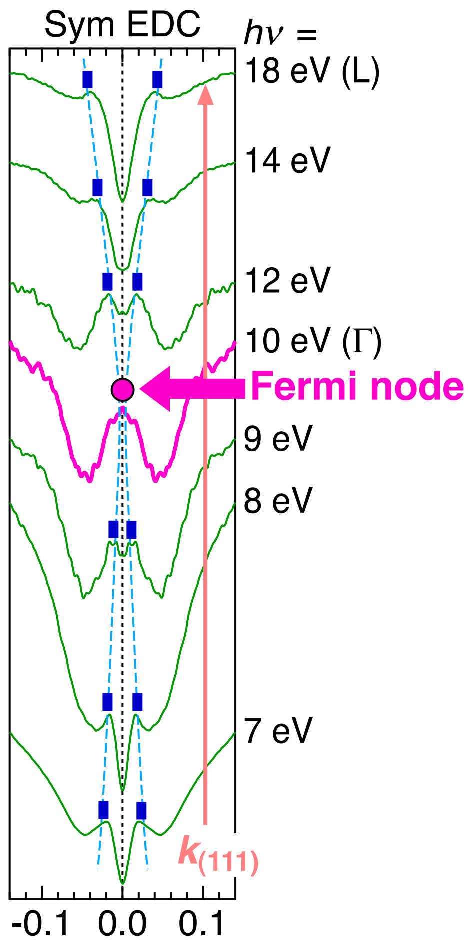
$Pr_2Ir_2O_7$

S. Nakatsuji

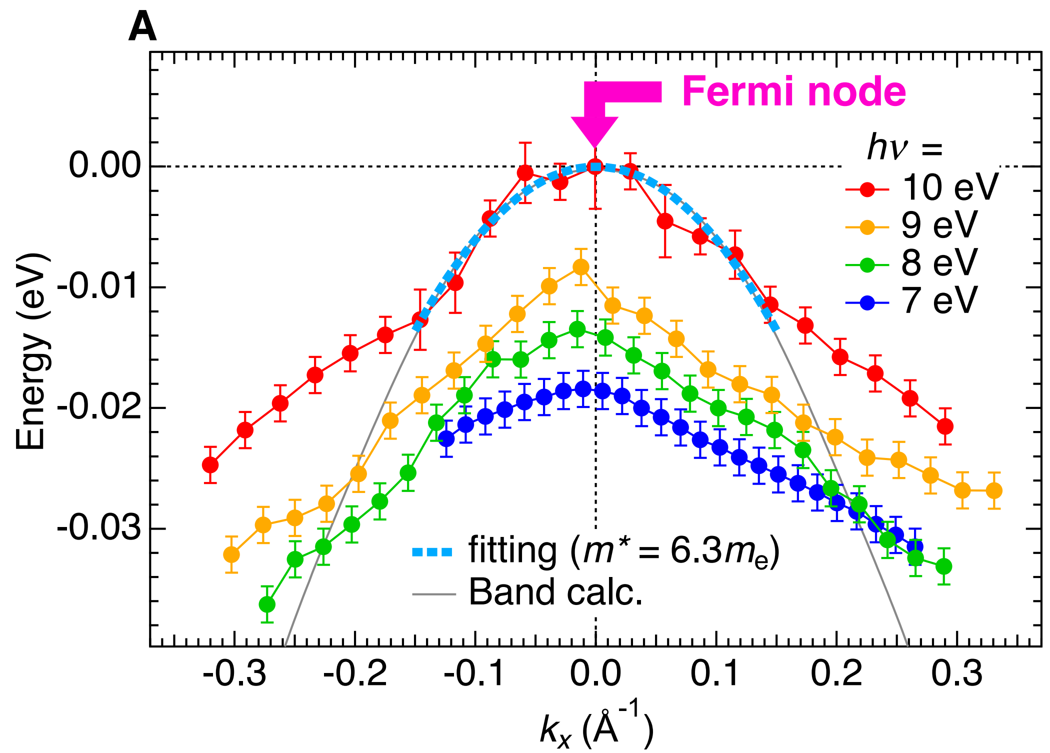
T. Kondo

S. Shin





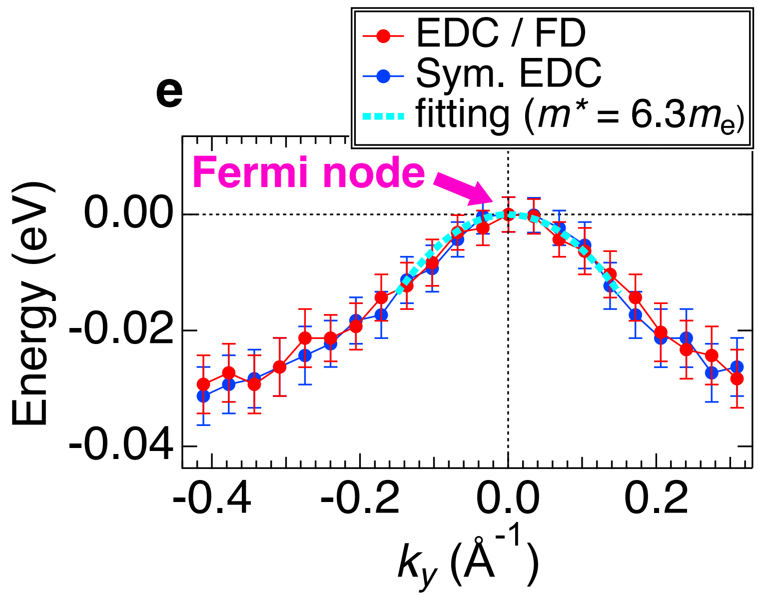
closest approach

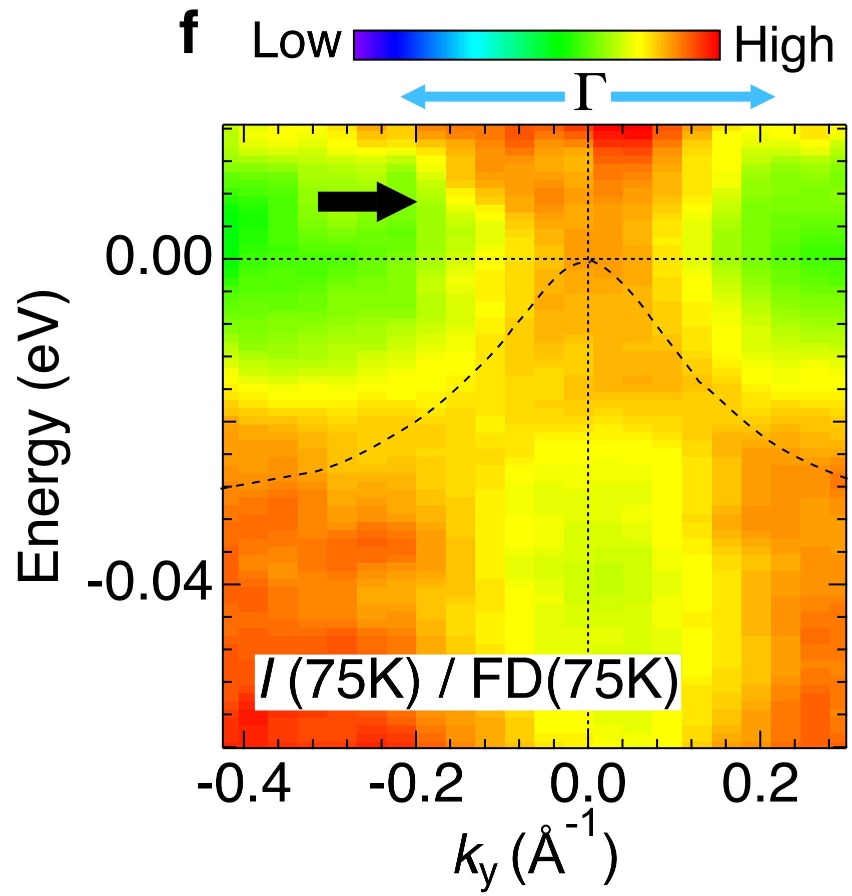


Valence band approaches the Fermi energy at few meV resolution

ARPES

$Pr_2Ir_2O_7$ S. Nakatsuji T. Kondo S. Shin





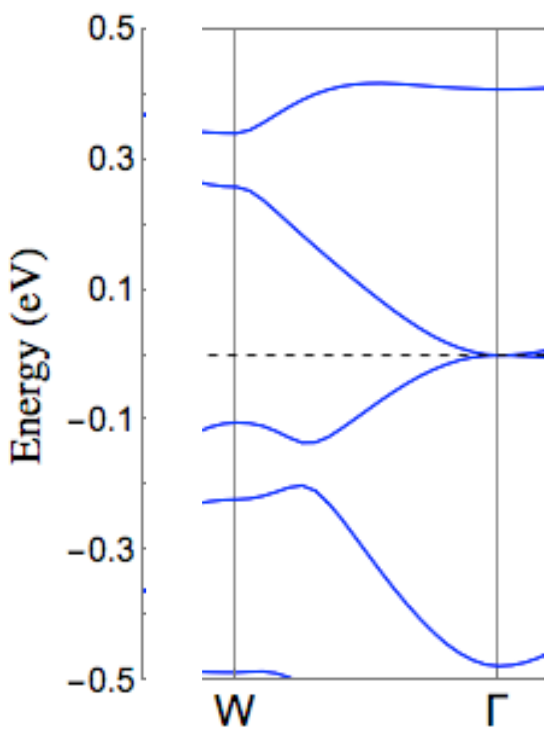
$Pr_2Ir_2O_7$

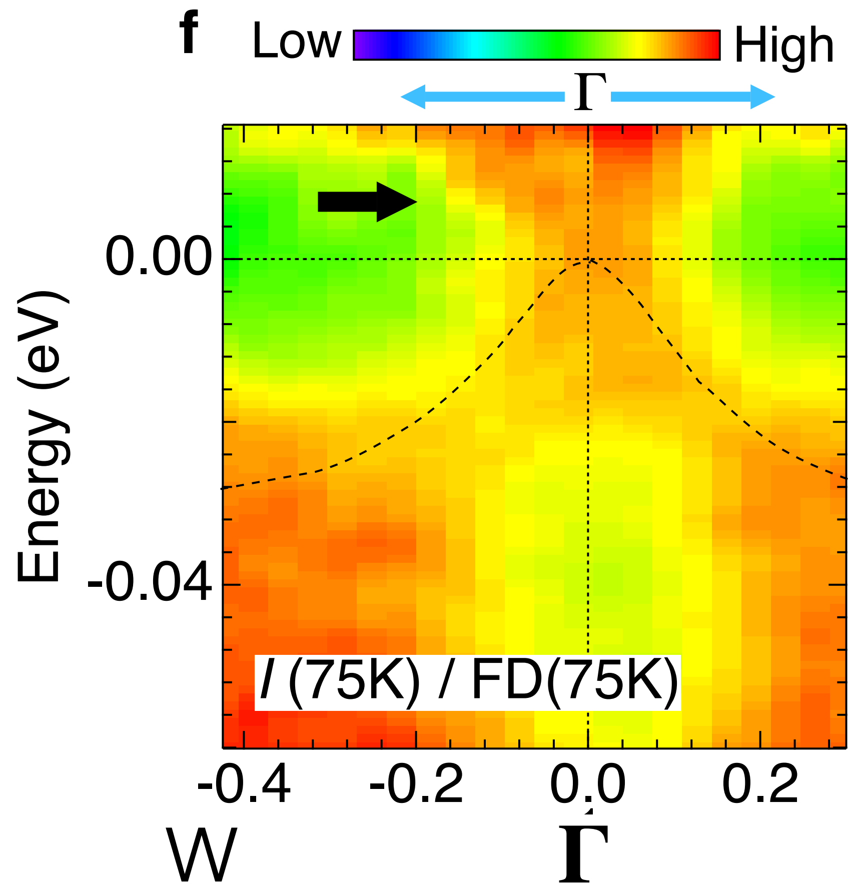
S. Nakatsuji

ARPES

T. Kondo

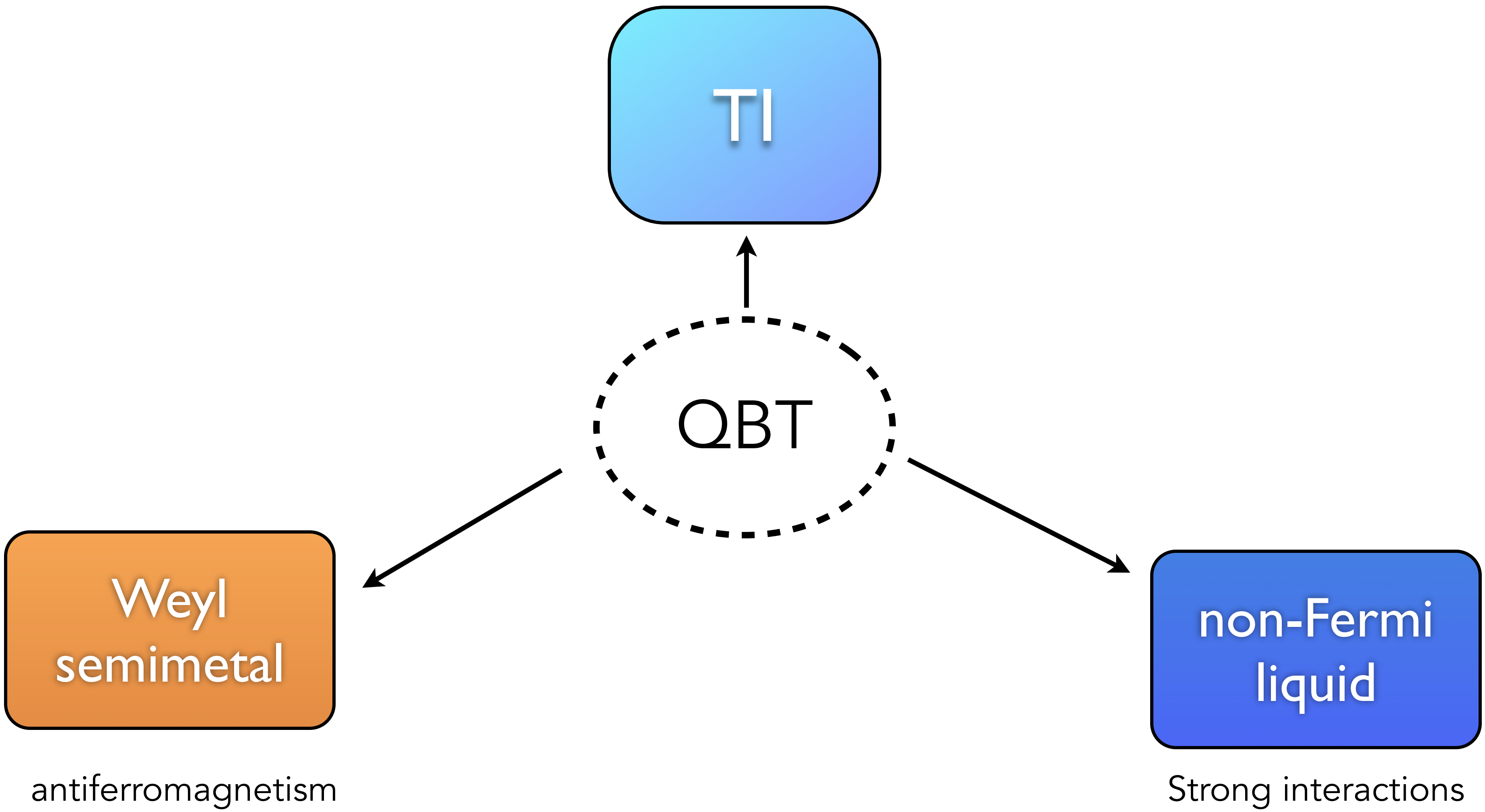
S. Shin



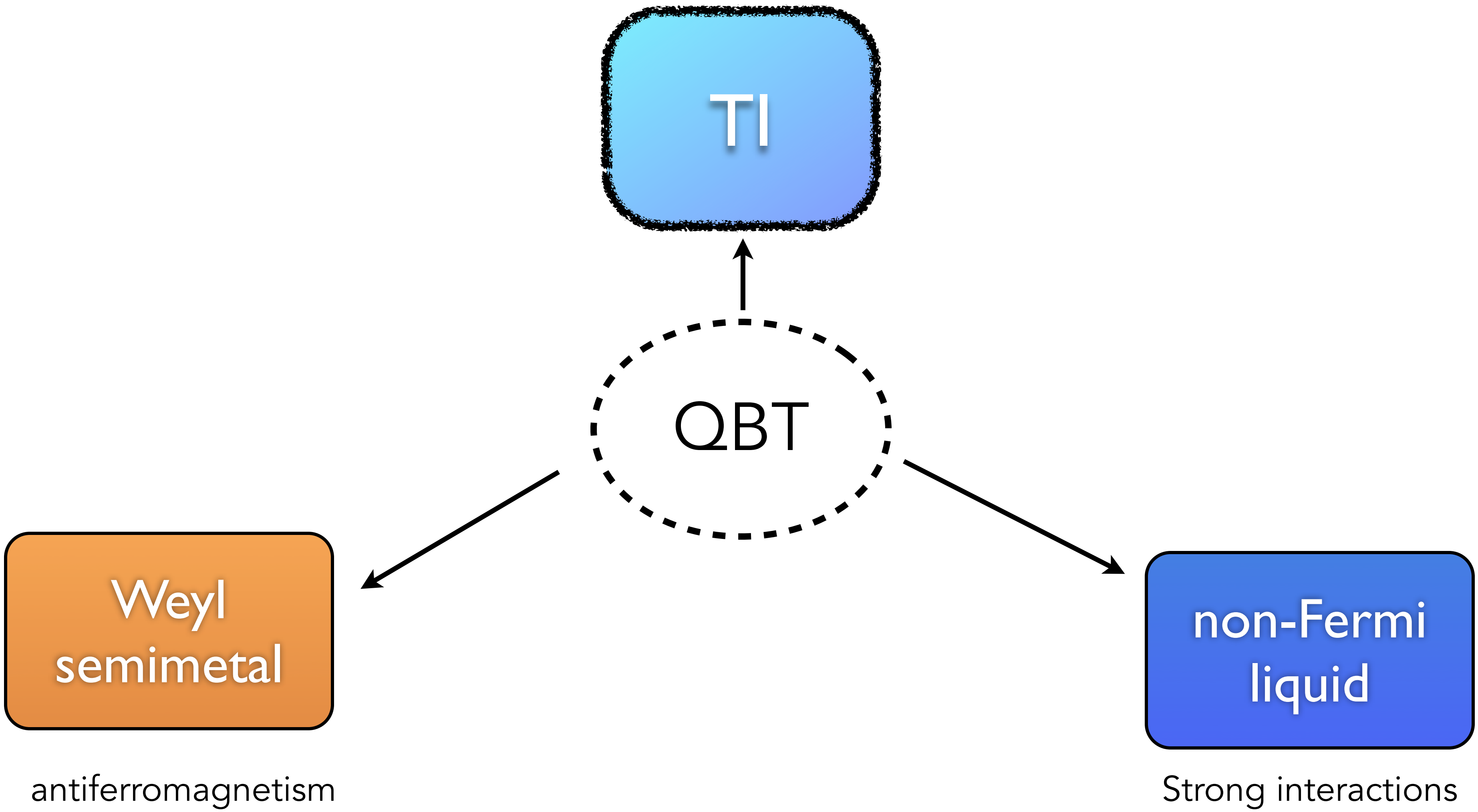


overall bandwidth ~ 5 times reduced

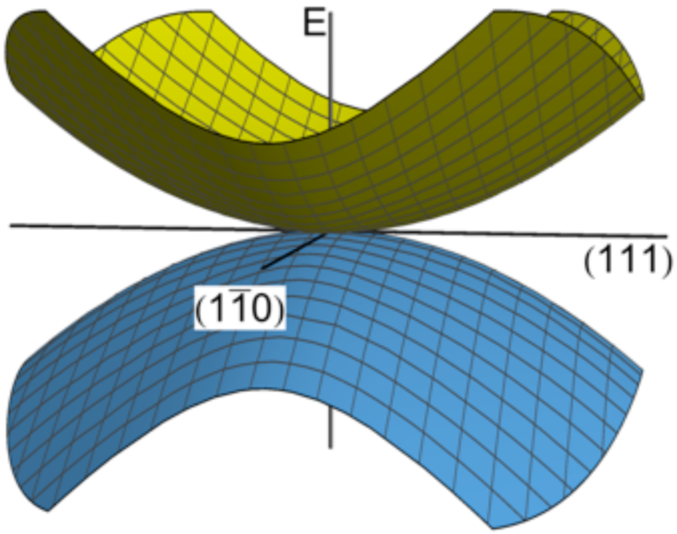
TI++


TI
QBT
Weyl semimetal
non-Fermi liquid
antiferromagnetism
Strong interactions

TI++


TI
QBT
Weyl semimetal
non-Fermi liquid
antiferromagnetism
Strong interactions

QBT to TI



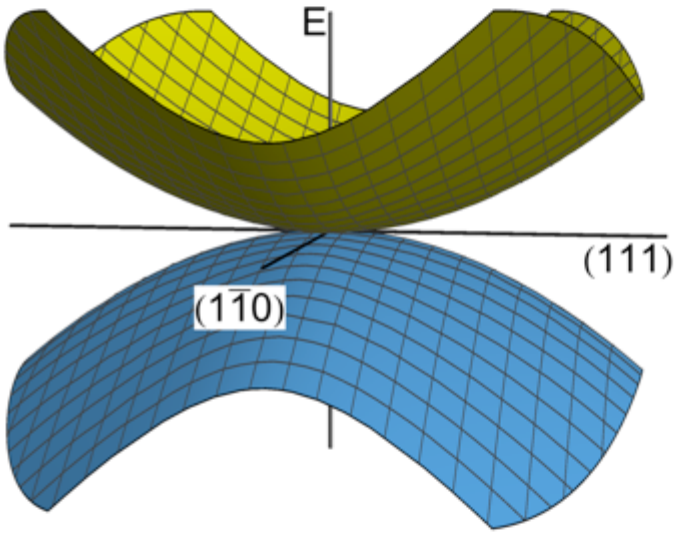
(111)
compression

???

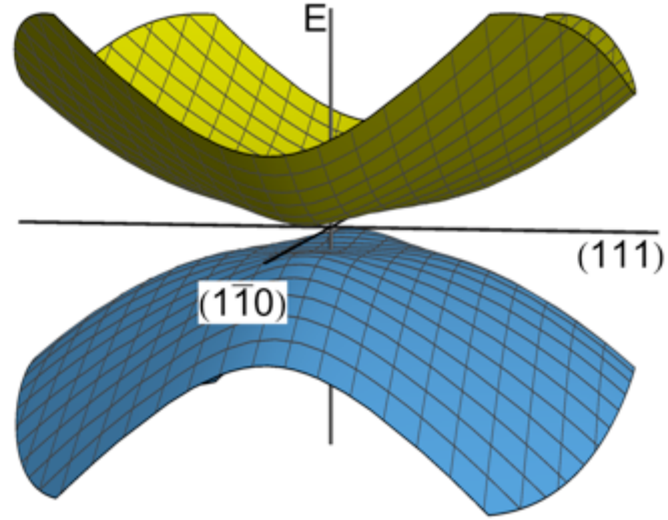
$$\mathcal{H}_0(k) = \frac{d_a(k)}{2m}\Gamma^a + \frac{k^2}{2M_0} + \frac{d_4(k)\Gamma^4 + d_5(k)\Gamma^5}{2M_c}$$

$$+\varepsilon\,\Gamma^5$$

QBT to TI



(111)
compression



$$\mathcal{H}_0(k) = \frac{d_a(k)}{2m}\Gamma^a + \frac{k^2}{2M_0} + \frac{d_4(k)\Gamma^4 + d_5(k)\Gamma^5}{2M_c}$$

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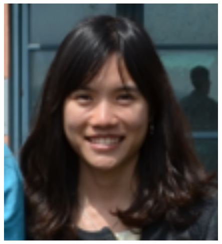
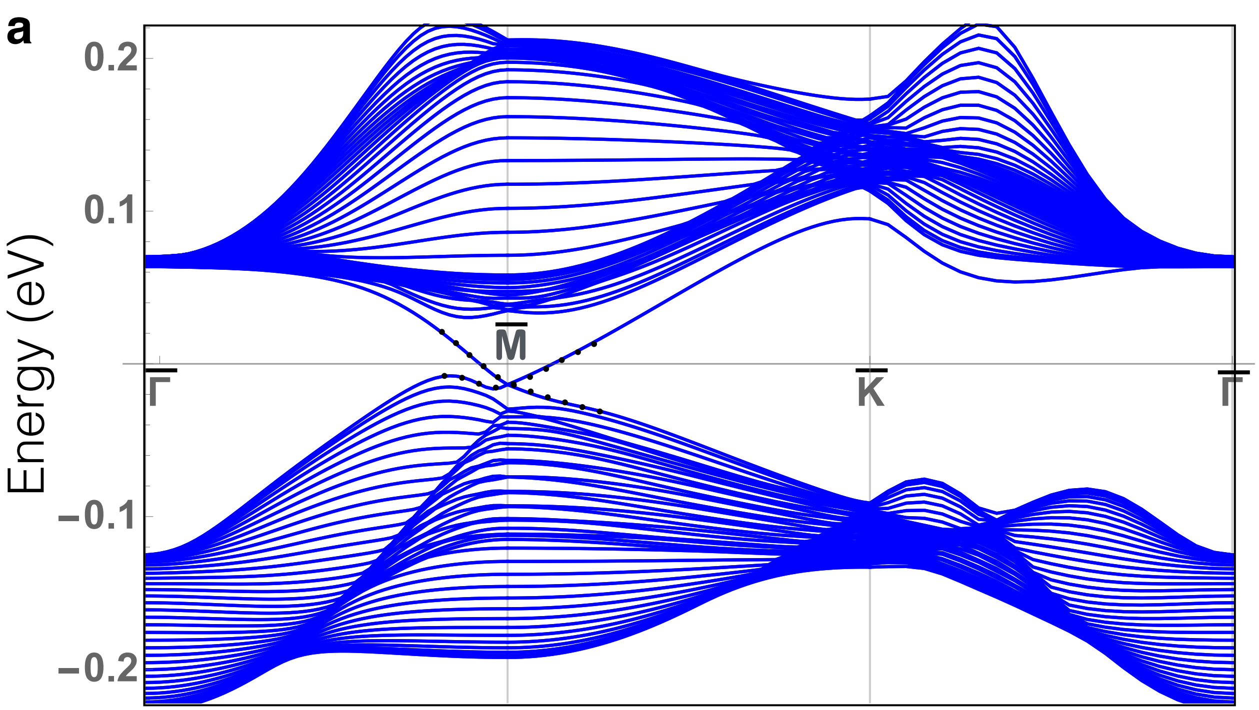
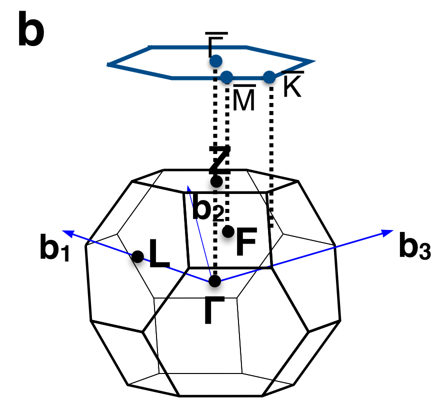
TI



Topological Insulator

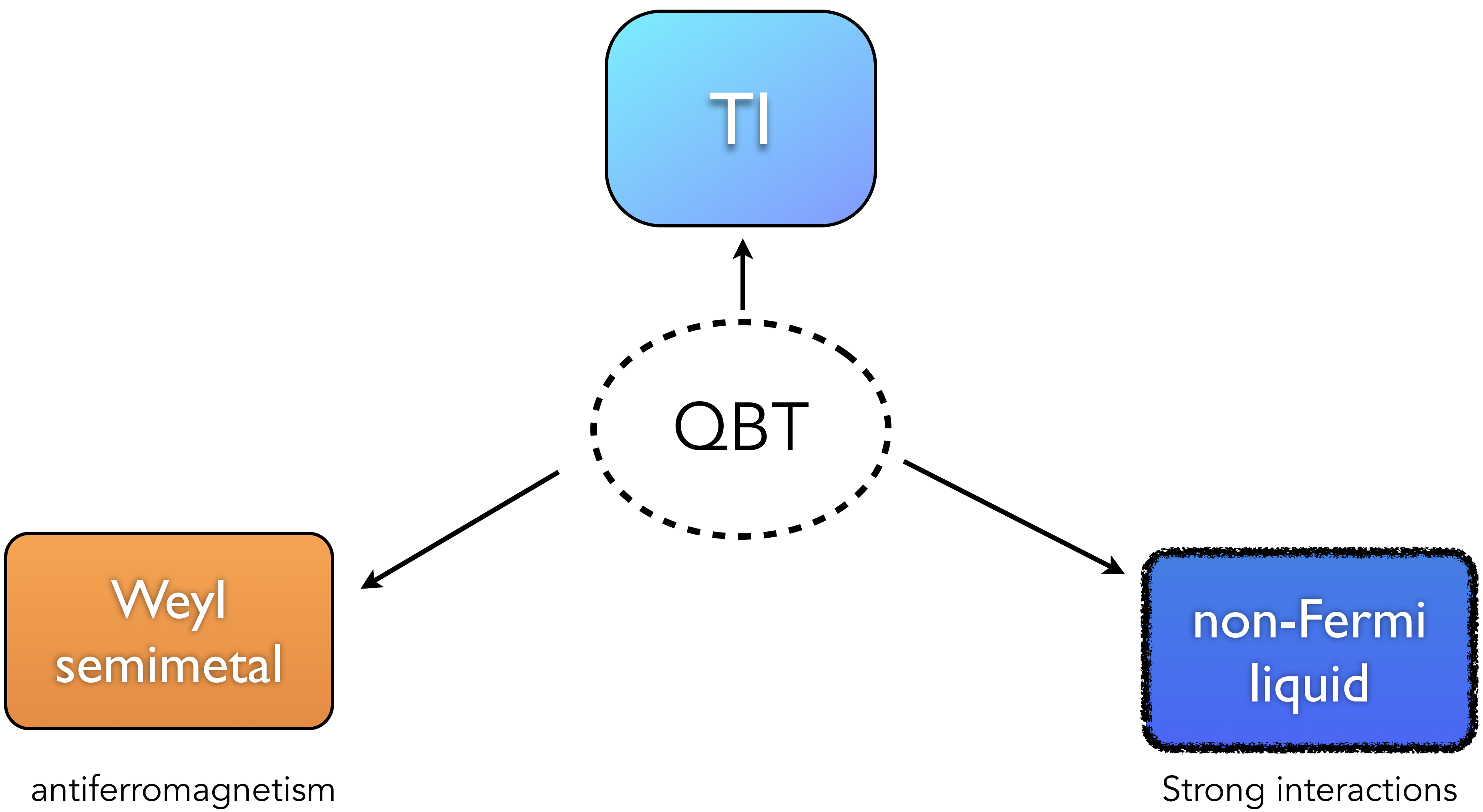
(111) compressive strain

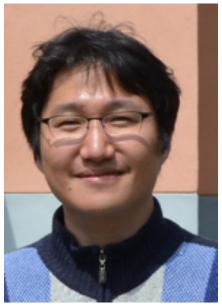




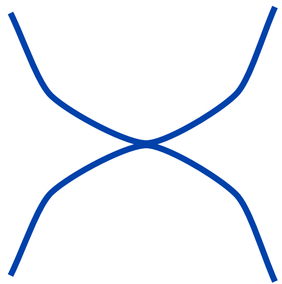
3 surface Dirac cones

TI++


TI
QBT
Weyl semimetal
non-Fermi liquid
antiferromagnetism
Strong interactions



LAB phase



+ Coulomb = NFL

POSSIBLE EXISTENCE OF SUBSTANCES INTERMEDIATE BETWEEN METALS AND DIELECTRICS

A. A. ABRIKOSOV and S. D. BENESLAVSKIĬ

L. D. Landau Institute of Theoretical Physics

Submitted April 13, 1970

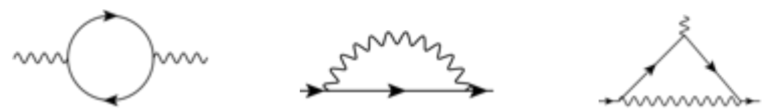
Zh. Eksp. Teor. Fiz. 59, 1280—1298 (October, 1970)

The question of the possible existence of substances having an electron spectrum without any energy gap and, at the same time, not possessing a Fermi surface is investigated. First of all the question of the possibility of contact of the conduction band and the valence band at a single point is investigated within the framework of the one-electron problem. It is shown that the symmetry conditions for the crystal admit of such a possibility. A complete investigation is carried out for points in reciprocal lattice space with a little group which is equivalent to a point group, and an example of a more complicated little group is considered. It is shown that in the neighborhood of the point of contact the spectrum may be linear as well as quadratic.

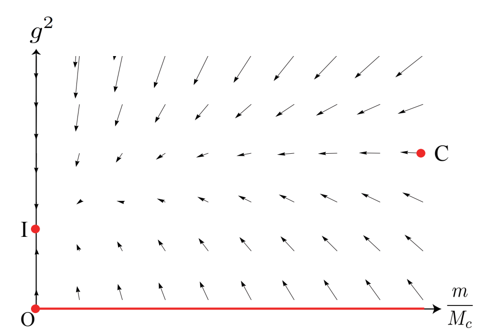
The role of the Coulomb interaction is considered for both types of spectra. In the case of a linear dispersion law a slowly varying (logarithmic) factor appears in the spectrum. In the case of a quadratic spectrum the effective interaction becomes strong for small momenta, and the concept of the one-particle spectrum turns out to be inapplicable. The behavior of the Green's functions is determined by similarity laws analogous to those obtained in field theory with strong coupling and in the neighborhood of a phase transition point of the second kind (scaling). Hence follow power laws for the electronic heat capacity and for the momentum distribution of the electrons.

QFT

$$S_L = \int d\tau d^d x \left\{ \psi^\dagger \left[\partial_\tau - ie\,\varphi + \hat{\mathcal{H}}_0 \right] \psi + \frac{c_0}{2} (\partial_i \varphi)^2 \right\}$$

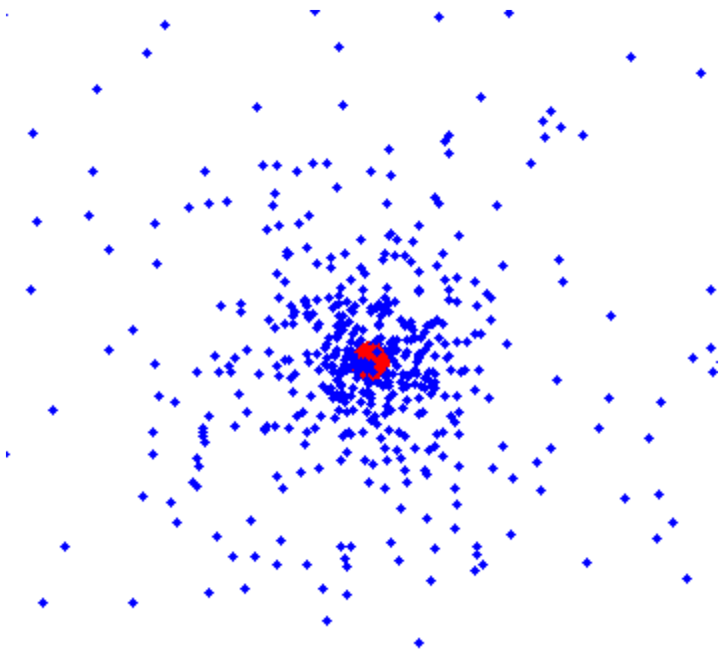


stable, NFL fixed point



"Luttinger-Abrikosov-Beneslavskii" phase

Screening



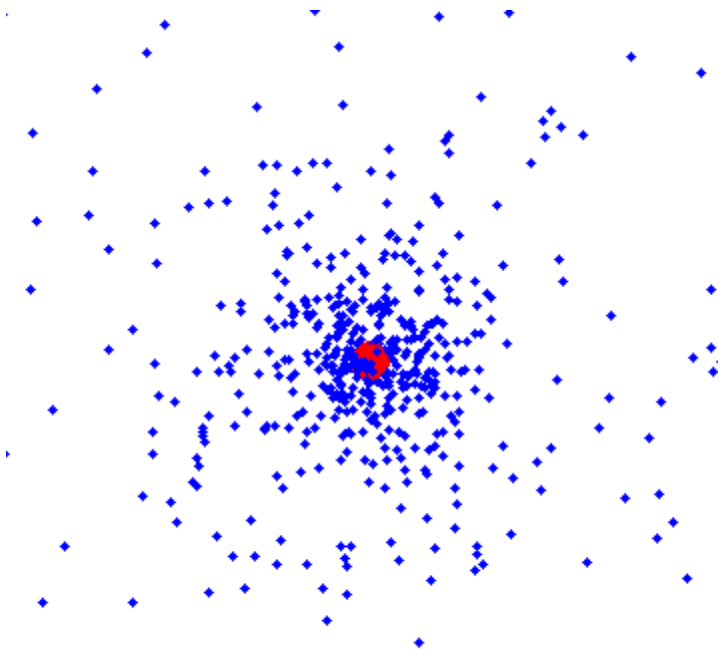
usual metal

$$V(q) = \frac{1}{\frac{q^2}{4\pi e^2} + \frac{\partial n}{\partial \mu}}$$

$$V(r) = \frac{e^2}{r} \to \frac{e^2}{r} e^{-r/\lambda}$$

$$\lambda_{TF}^{-2} = 4\pi e^2 \frac{\partial n}{\partial \mu}$$

Screening



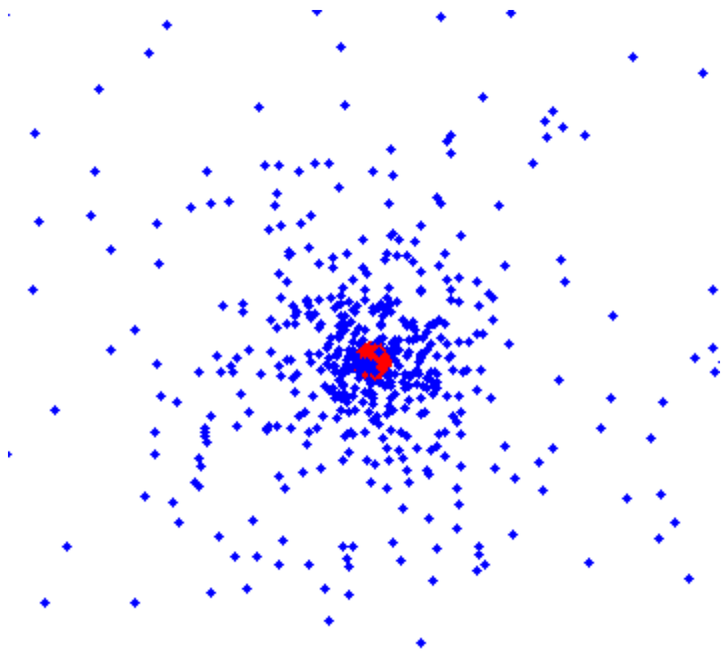
quadratic band touching

$$V(q) = \frac{1}{\frac{q^2}{4\pi e^2} + \frac{\partial n}{\partial \mu}}$$

$$\frac{\partial n}{\partial \mu} \sim \sqrt{\epsilon} \sim q$$

$$V(r) = \frac{e^2}{r} \rightarrow \frac{k}{r^2}$$

Screening



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$$V(q) = \frac{1}{\frac{q^2}{4\pi e^2} + \frac{\partial n}{\partial \mu}}$$

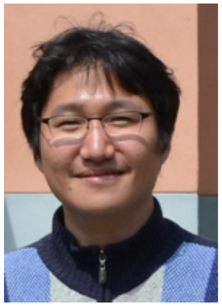
$$\frac{\partial n}{\partial \mu} \sim \sqrt{\epsilon} \sim q$$

$$V(r) = \frac{e^2}{r} \to \frac{k}{r^2}$$

Quantum mechanics

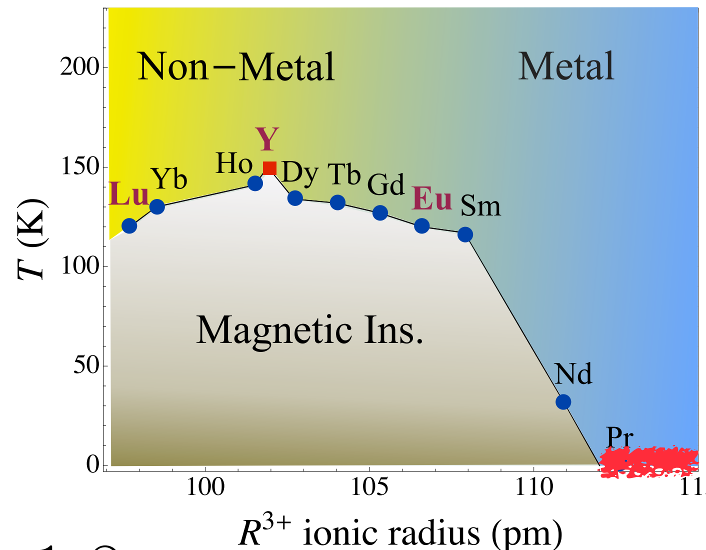
$$\left\{ -\frac{1}{2m}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right] + \frac{k}{r^2} \right\} \psi(r) = E\psi(r)$$

scale invariance!



NFL phase

Proper analysis:
large N or
epsilon
expansion



NFL

$$\omega \sim k^z \quad z \approx 1.8$$

scaling,
e.g.

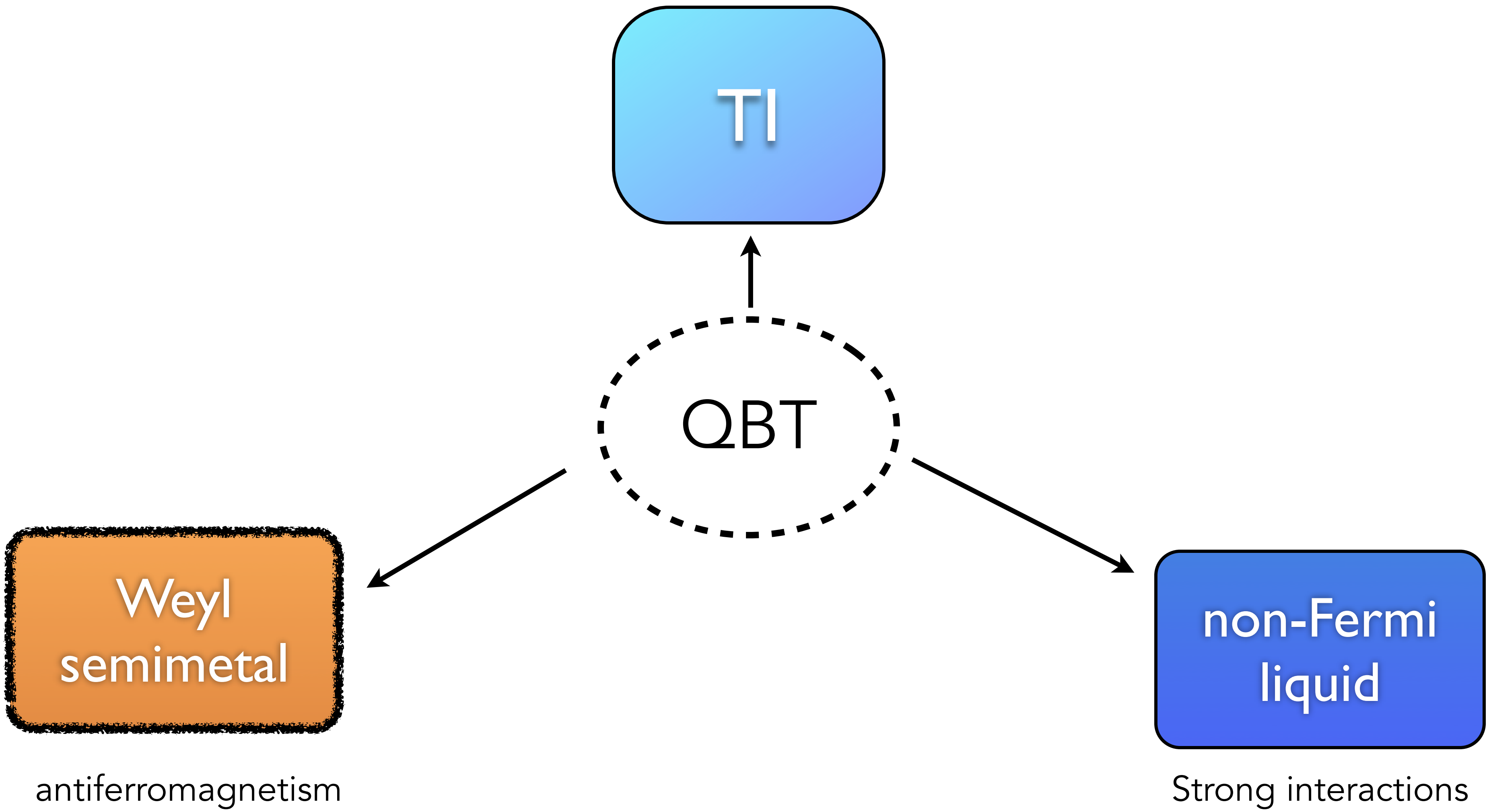
$$c_v \sim T^{d/z} \approx T^{1.7}$$

$$\sigma(\omega) \sim \omega^{1/z}$$

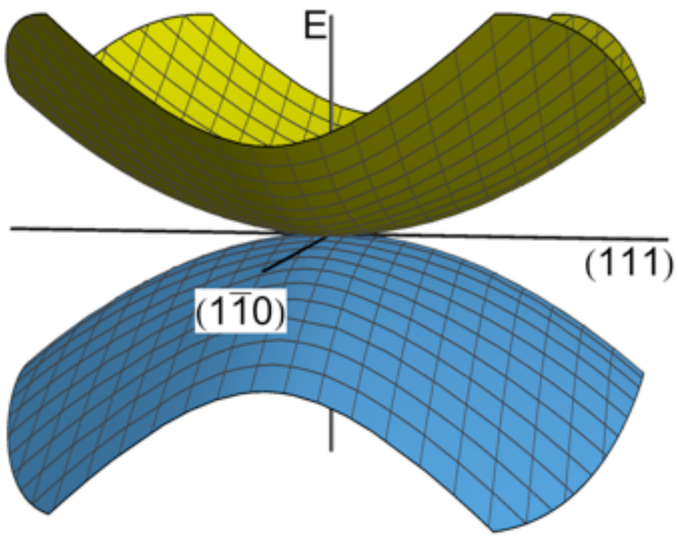
"Luttinger-Abrikosov-Beneslavskii" phase

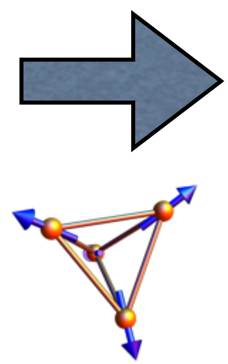
EG Moon, C. Xu, YB Kim, LB, PRL (2013)

TI++


TI
QBT
Weyl semimetal
non-Fermi liquid
antiferromagnetism
Strong interactions

Weyl semimetal

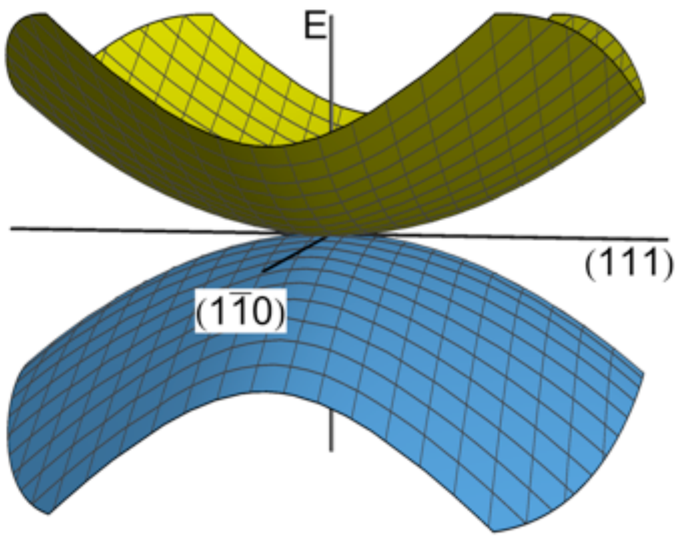


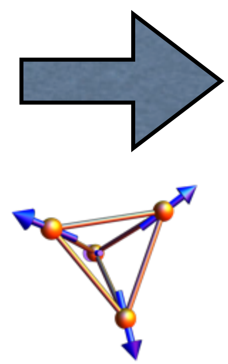


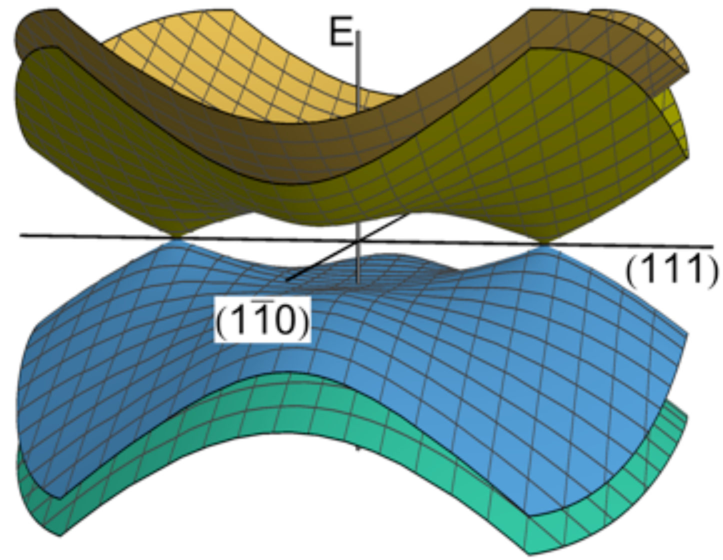
???

$$\mathcal{H}_0(k) = \frac{d_a(k)}{2m}\Gamma^a + \frac{k^2}{2M_0} + \frac{d_4(k)\Gamma^4 + d_5(k)\Gamma^5}{2M_c}$$
$$+\, i\phi\,\Gamma^4\Gamma^5$$

Weyl semimetal



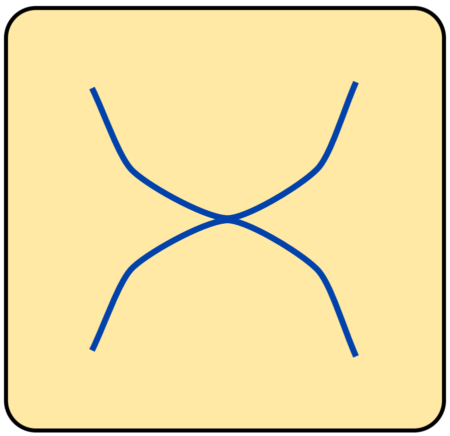




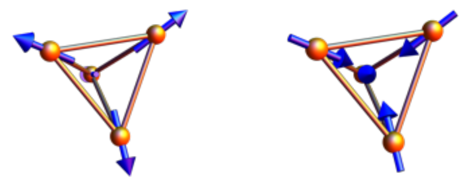
$$\mathcal{H}_0(k) = \frac{d_a(k)}{2m}\Gamma^a + \frac{k^2}{2M_0} + \frac{d_4(k)\Gamma^4 + d_5(k)\Gamma^5}{2M_c}$$
$$+ i\phi\,\Gamma^4\Gamma^5$$

antiferromagnetic Weyl semimetal

Field theory



$+$



$= ??$

ϕ

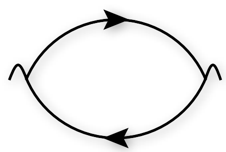
$$S = \int d\tau d^3x \left[\overline{\psi}_a (\partial_\tau + \hat{\mathcal{H}}_0)\psi_a + \frac{g}{\sqrt{N}} \phi \, \overline{\psi}_a \mathsf{M} \, \psi_a + \frac{r}{2}\phi^2 \right]$$
$$+ \frac{ie}{\sqrt{N}} \varphi \, \overline{\psi}_a \psi_a + \frac{1}{2}(\nabla \varphi)^2$$

poor screening

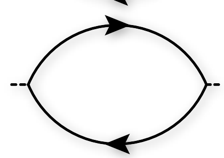
Approach

large N_{fermion} expansion & RG

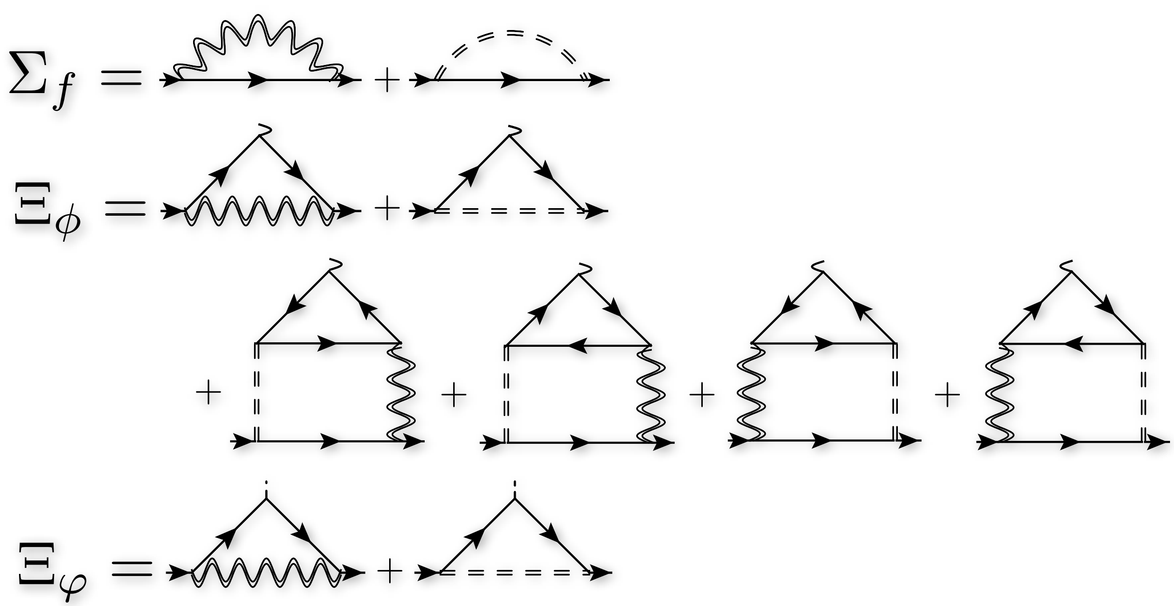
all-in-all-out order parameter

$\Sigma_\phi =$  $\sim |\mathbf{k}|\,|\ln c_1/c_2\,|f_\phi(\hat{\mathbf{k}}) + \sqrt{\omega_n}\,C \quad \gg \overbrace{\mathbf{k}^2 + \omega_n^2}^{\mathcal{G}_{0;b}^{-1}}$

Coulomb interactions

$\Sigma_\varphi =$  $\sim |\mathbf{k}|\,|\ln c_1/c_2\,|f_\varphi(\hat{\mathbf{k}}) \quad \gg \mathbf{k}^2$

bare



$\propto 1/N_{\text{fermion}} \times \ln\Lambda$

<u>RG:</u> calculate "only" the coefficient of lnΛ

Quantum criticality

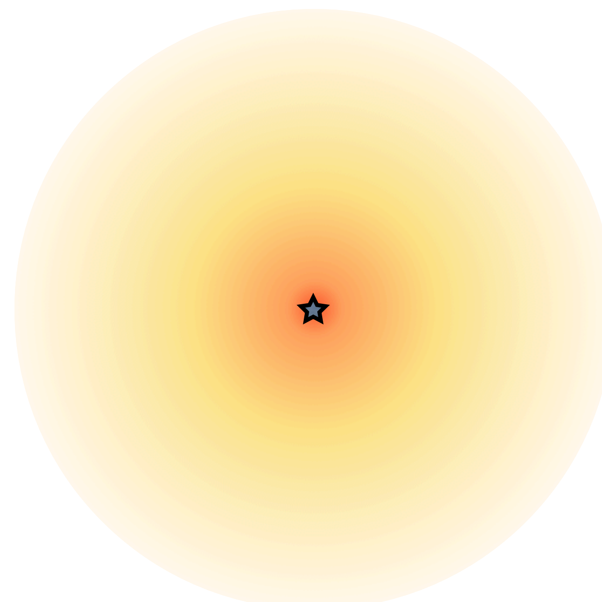
- Stable fixed point with unusual exponents: extreme deviations from MFT

e.g. $\langle\phi\rangle \sim (r_c - r)^2$

(x logs)

wide QC regime $z \approx 2$

$\nu \approx 1$



Semimetal

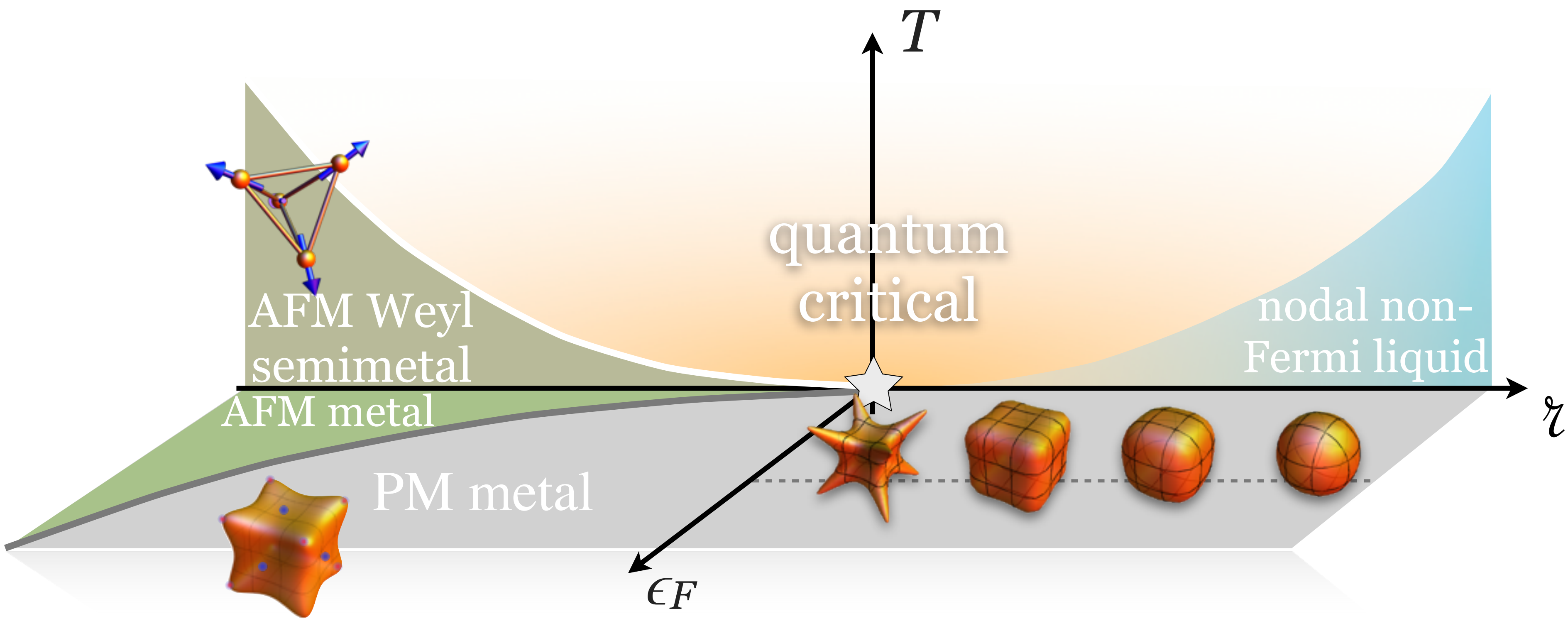
$\chi^{-1} \sim q + \sqrt{|\omega|}$

matched to electrons

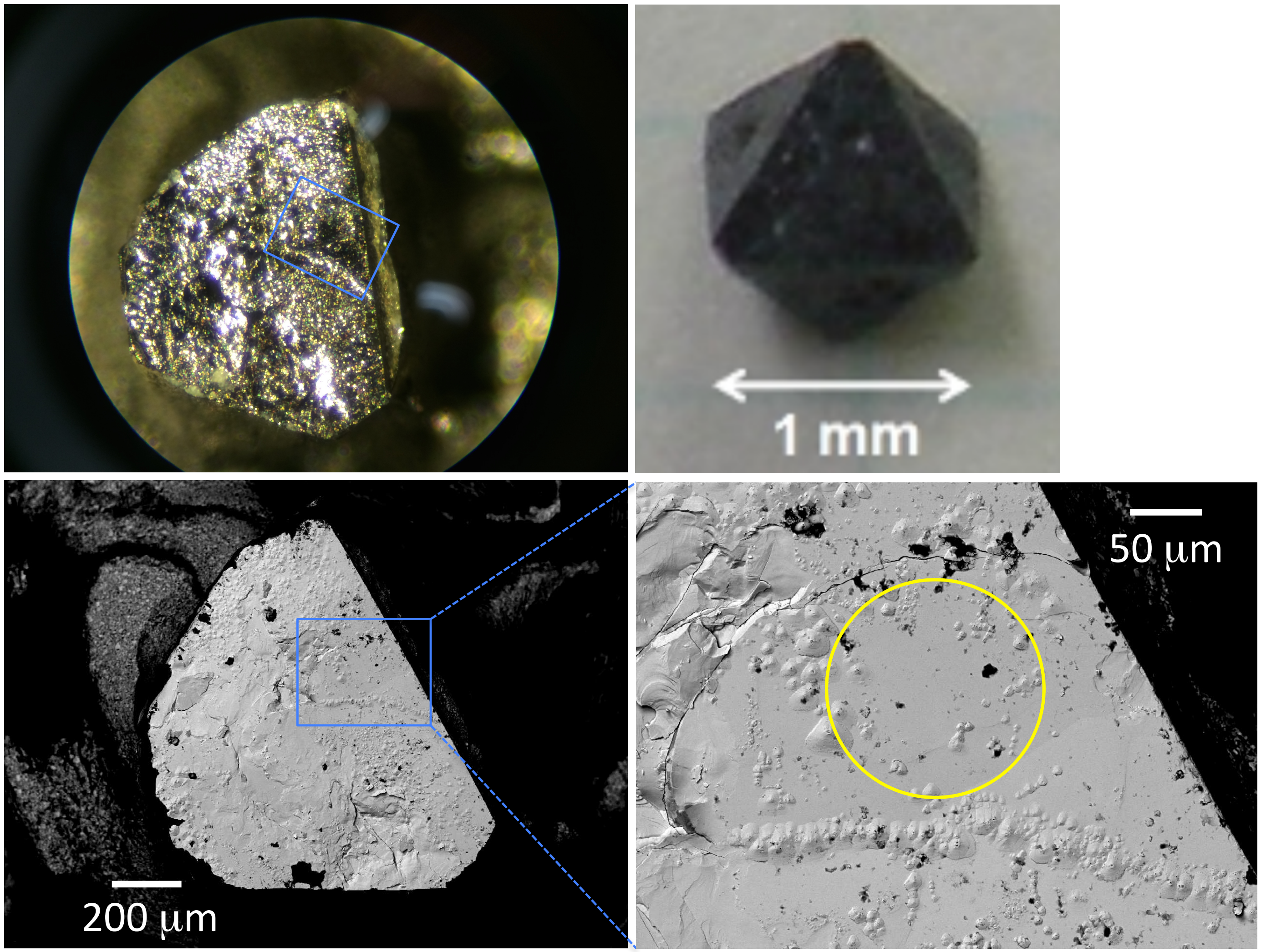
electrons scatter strongly

Quantum criticality

- QBT leads to extremely non-classical QCP

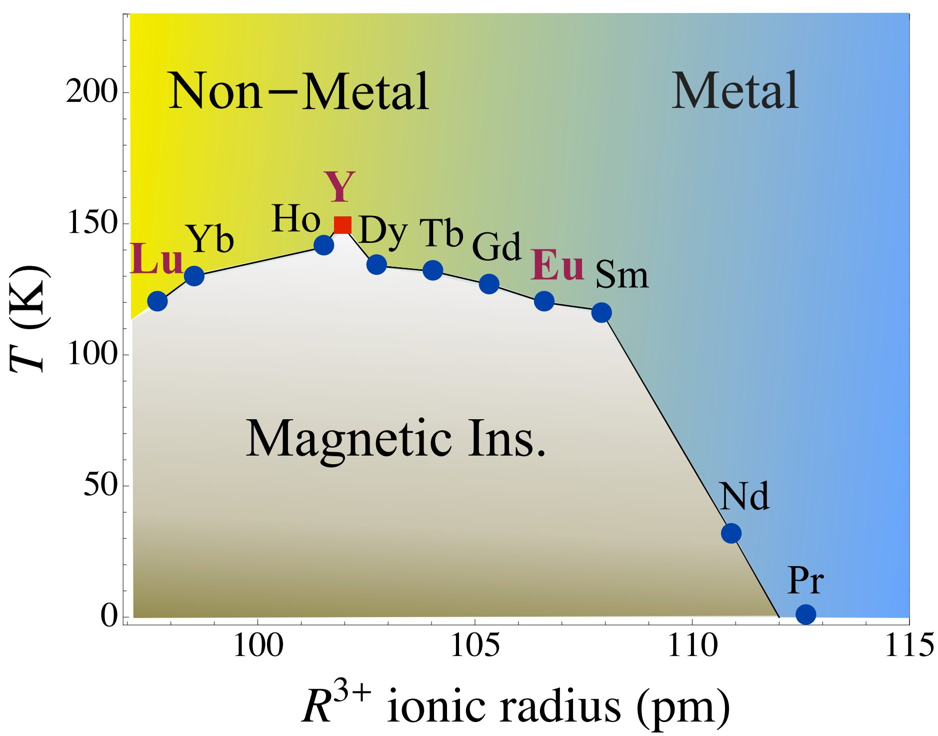


L. Savary, EG Moon, LB, PRX, 2014


1 mm
200 μm
50 μm

Pyrochlore iridates

- Weyl semimetal?

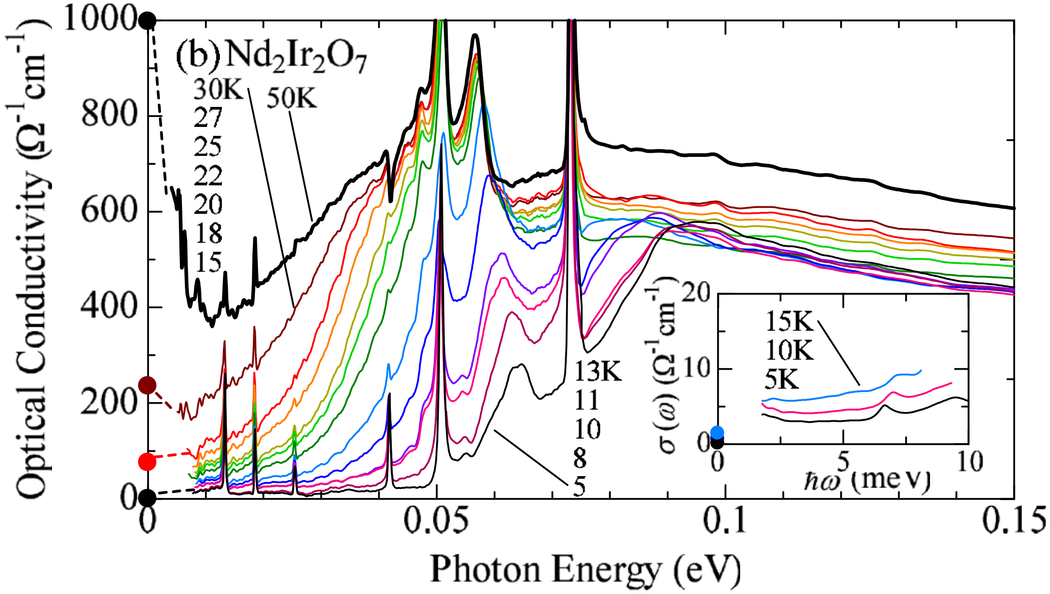


Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

Best candidate should be $Nd_2Ir_2O_7$

Weyl not?

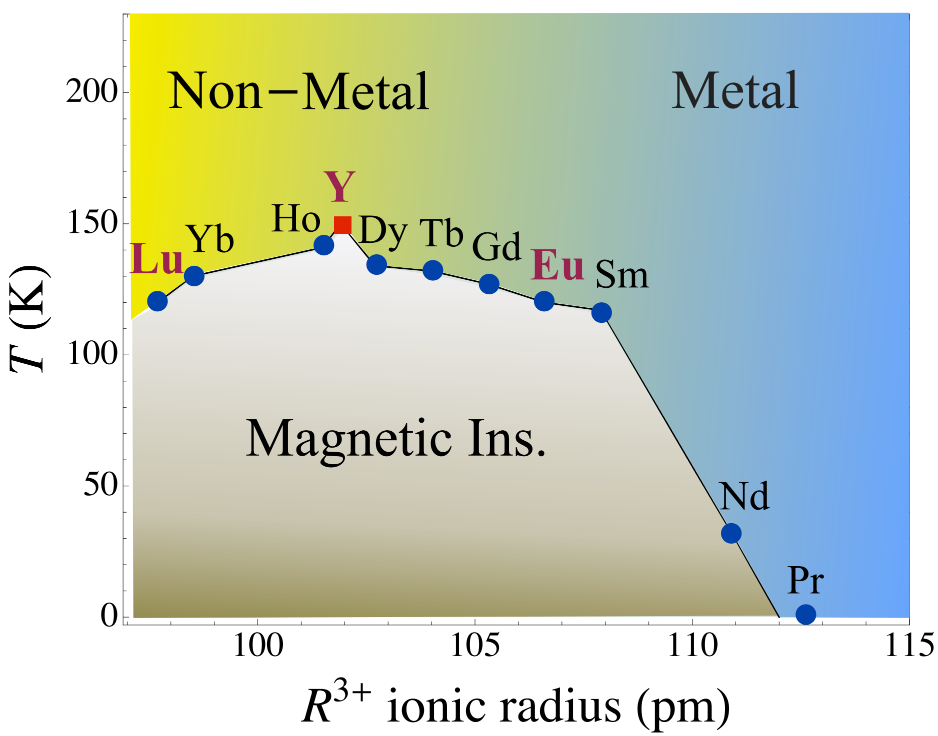
K. Ueda *et al*, 2012



Clear charge gap ~ 45meV

Pyrochlore iridates

- Continuous magnetic/metal-insulator transitions

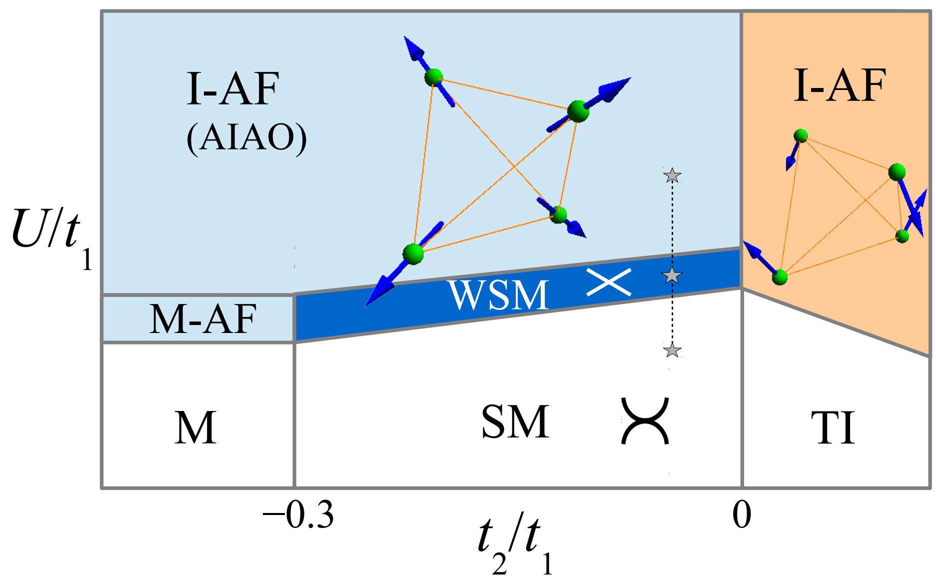


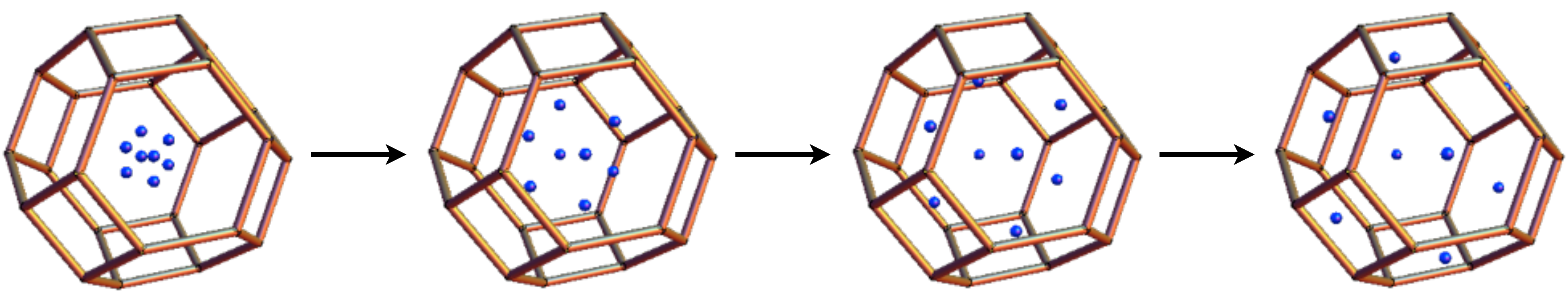
Yanagashima+Maeno, JPSJ 2001
K. Matsuhira et al, JPSJ 2011
W. Witczak-Krempa et al, ARCMP 2013

Puzzling things:

- Already a gap for weakest ordering?
- T_c=30K, gap >500K
- Why such low scales when U~t~10^4K?

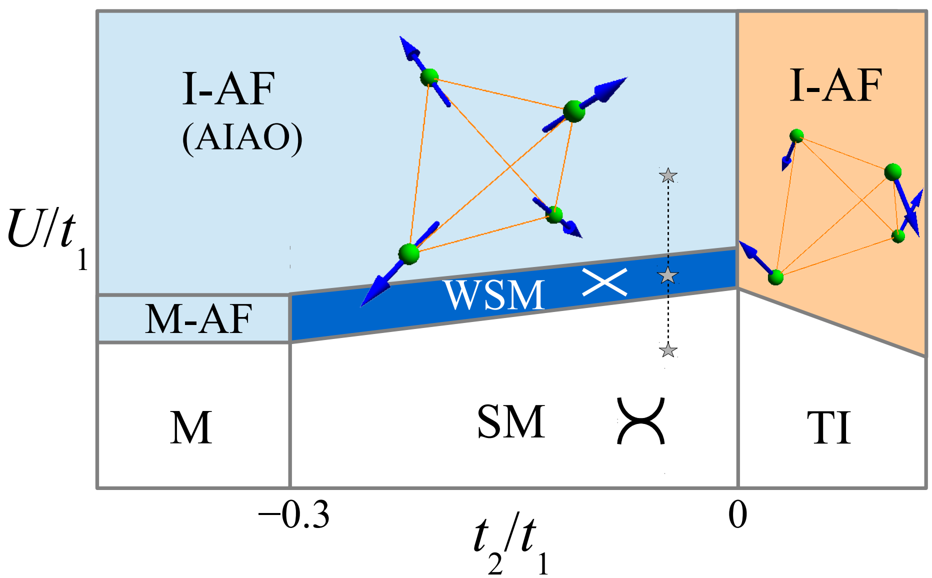
Weyl not?

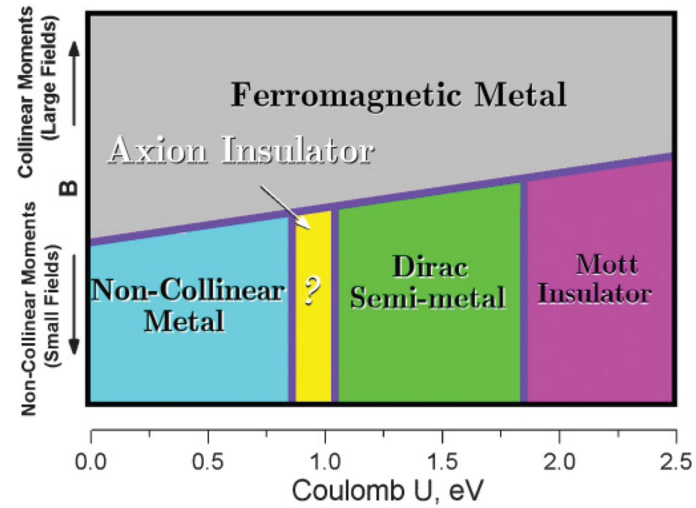


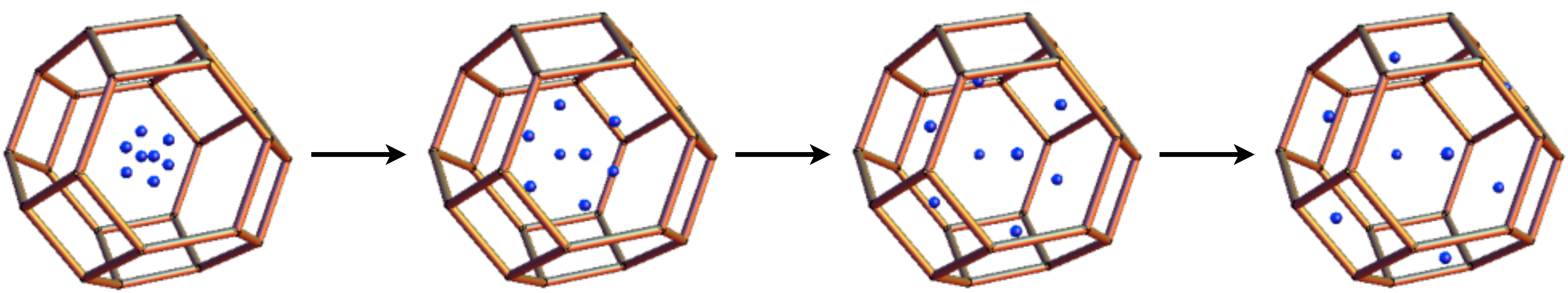


Weyl points move to zone boundary and annihilate with increasing order?

Weyl not?







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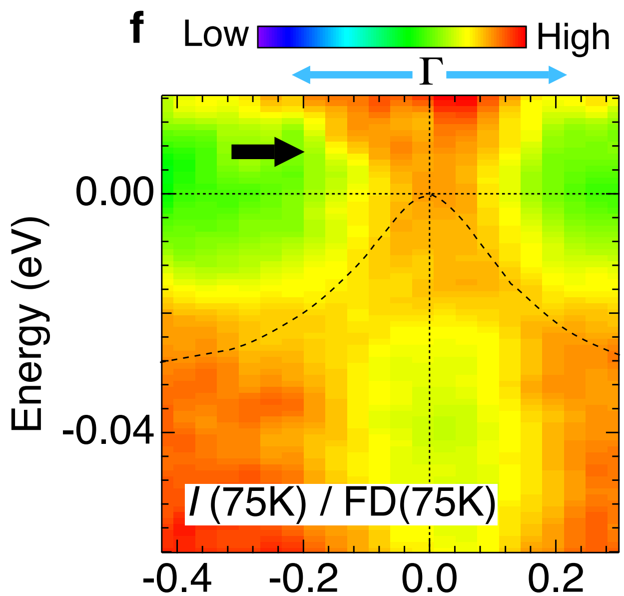
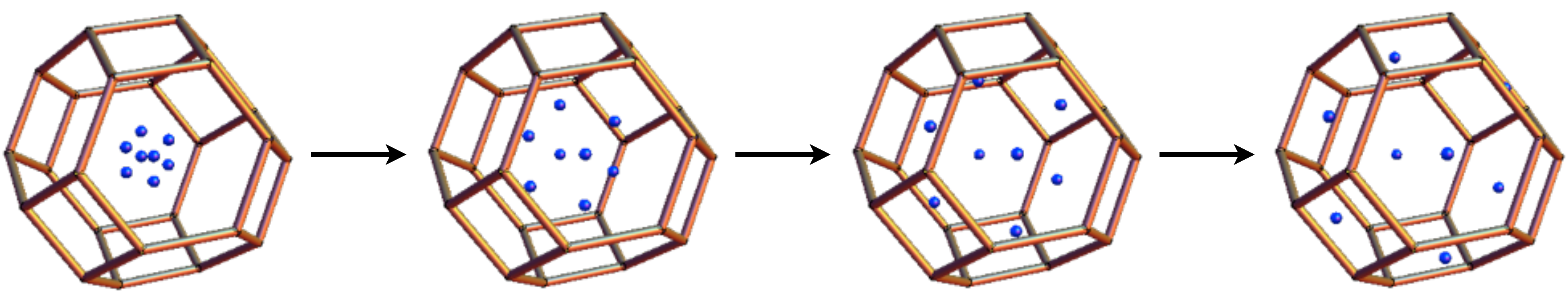
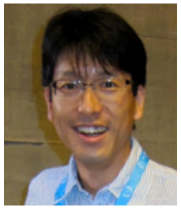


maybe bandwidth reduction
makes this possible



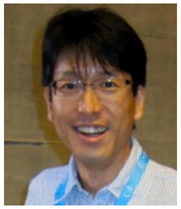
Weyl points move to zone boundary and annihilate with increasing order?



unpublished

Metal-insulator transition

very sensitive to stoichiometry



Metal-insulator transition

very sensitive to stoichiometry

field *close to (100)* kills
the insulating state

Metal-Insulator Transition

- Why only along (100)?
- Why such a small field?
- What is the nature of the metallic state?

Metal-Insulator Transition

- Why only along (100)?
- Why such a small field?
- What is the nature of the metallic state?

Due to Nd moments

Nd physics

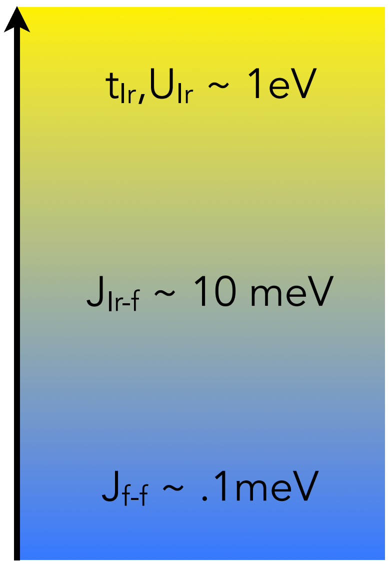
- Nd has large moment: ~2.3muB
- Similar to “spin ice” Ising moments?

Nd physics

- In detail it is quite distinct from spin ice. Simple Ising moments would have abrupt features for all orientations.

Physics

- Kondo lattice $$H = H_{Ir} + H_K + H_B$$



$$H_K = \sum_{ia} \vec{S}_i \cdot \mathsf{J}_{ia} \cdot \vec{\tau}_a$$

$$H_B = -\sum_i \vec{B} \cdot g_i \cdot \vec{S}_i - \sum_a \vec{B} \cdot g_a \cdot \vec{\tau}_a$$

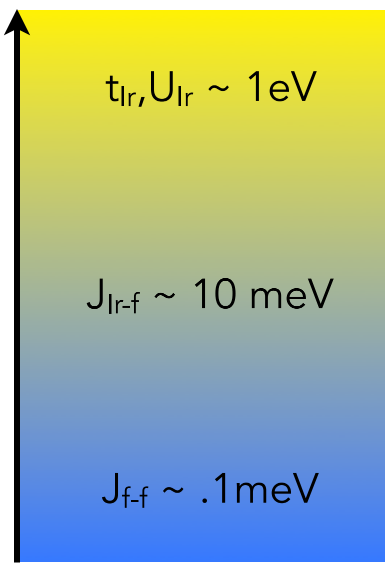
Ising-like moments

$$(g_a)_{\mu\nu} = g\hat{e}_\mu \delta_{\nu,3}$$

Octupolar-dipolar doublet:
Y.P. Huang *et al*

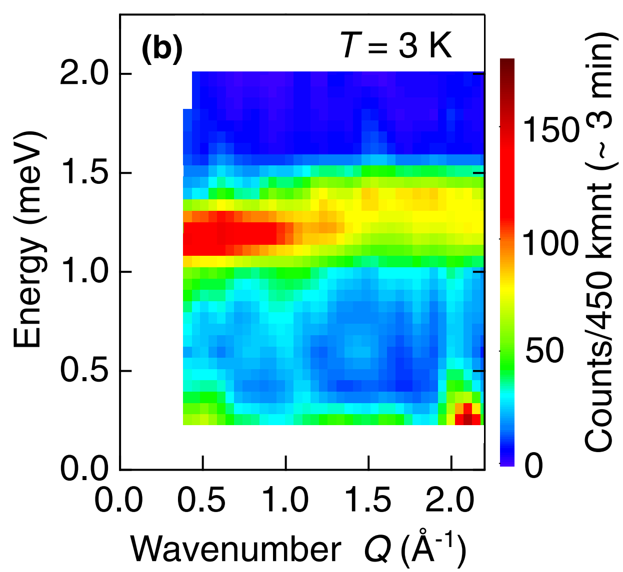
Physics

- Kondo lattice $H = H_{Ir} + H_K + H_B$



$$H_K = \sum_{ia} \langle \vec{S}_i \rangle \cdot \mathrm{J}_{ia} \cdot \vec{\tau}_a$$

gives effective field



Tomiyasu *et al, 2012*

Ising-like moments

Nd Zeeman splitting ~ 1.2meV

J probably larger as Ir ordered moment is small

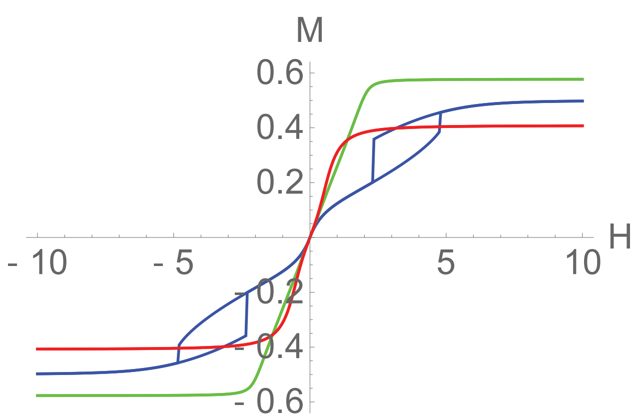
Magnetization

- Since magnetization is due to Nd, can integrate out Ir to obtain effective spin model

$$H_{Nd} = \sum_{<ij>} J_z \tau_i^z \tau_j^z + J_y \tau_i^y \tau_j^y + J_x \tau_i^x \tau_j^x + J_{xz}(\tau_i^x \tau_j^z + \tau_i^z \tau_j^x) \\ - A_H \sum_i \tau_i^z - g \sum_i \tau_i^z (\hat{n}_i \cdot \bar{H})$$

RKKY

exchange
+Zeeman fields

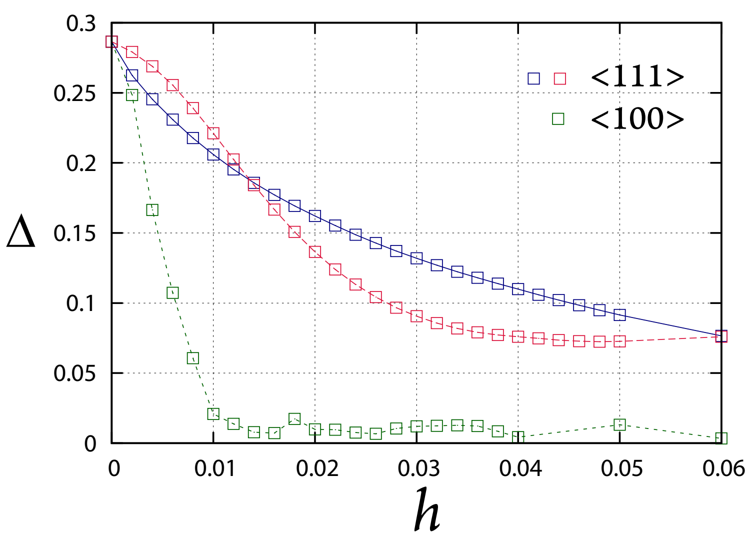


Explains M curves *if*

- Non-Ising terms substantial
- RKKY interactions are ferromagnetic

Anisotropy

- Intrinsic strong sensitivity of Nd to field direction is transferred to Ir



Hartree-Fock on Hubbard+Kondo lattice model

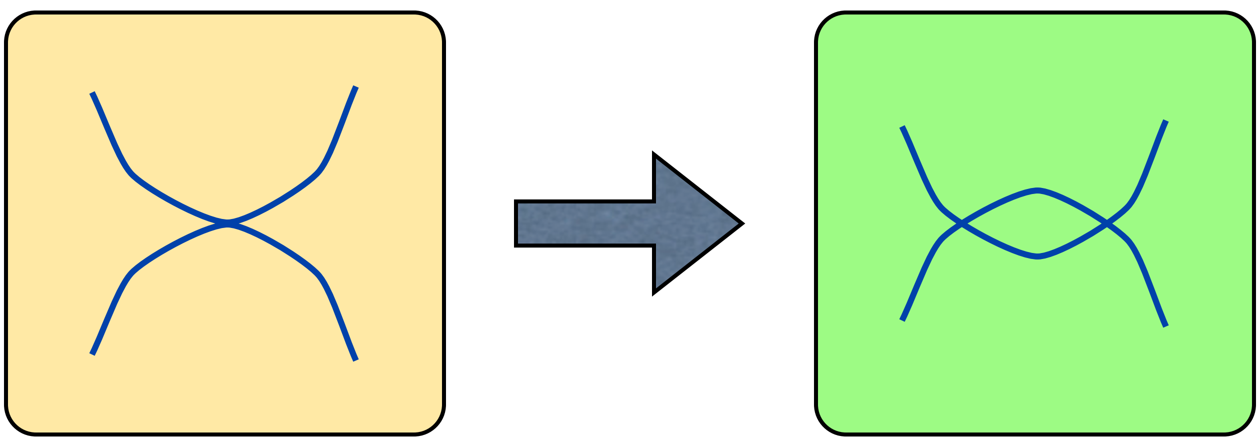
Kondo coupling completely overwhelms direct Zeeman field

Metal-Insulator Transition

- Why only along (100)?
- Why such a small field?
- What is the nature of the metallic state?

Weyl?

- Guess: field completely suppresses AIAO Ising order
- Like quadratic band touching with uniform field?



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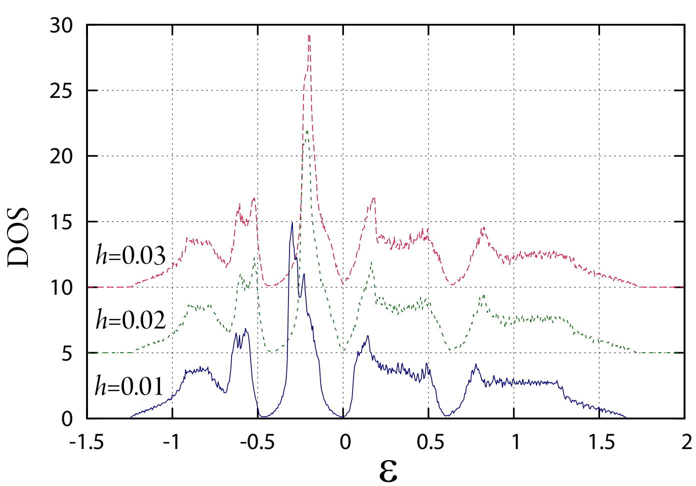
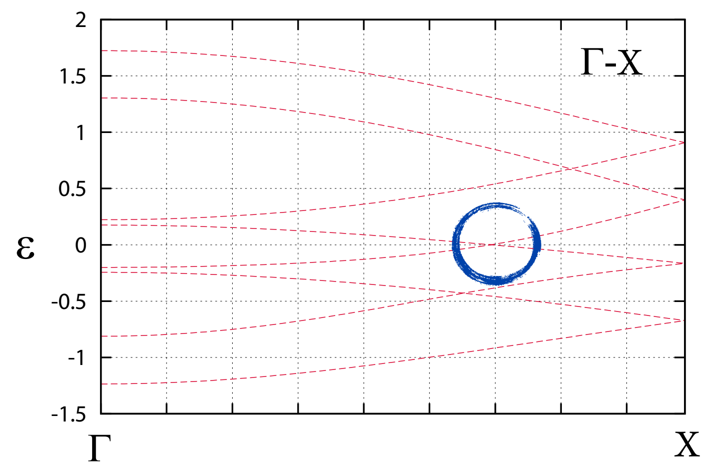
- Guess: field completely suppresses AIAO Ising order
- Like quadratic band touching with uniform field?





Weyl?

- Guess: field completely suppresses AIAO Ising order
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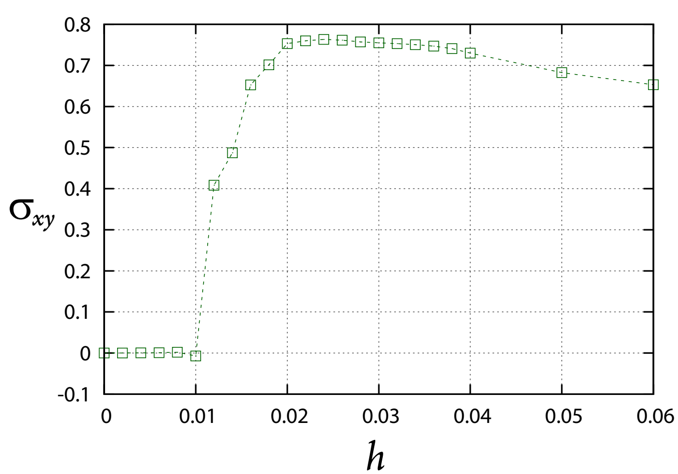

Simple model gives large Hall conductivity

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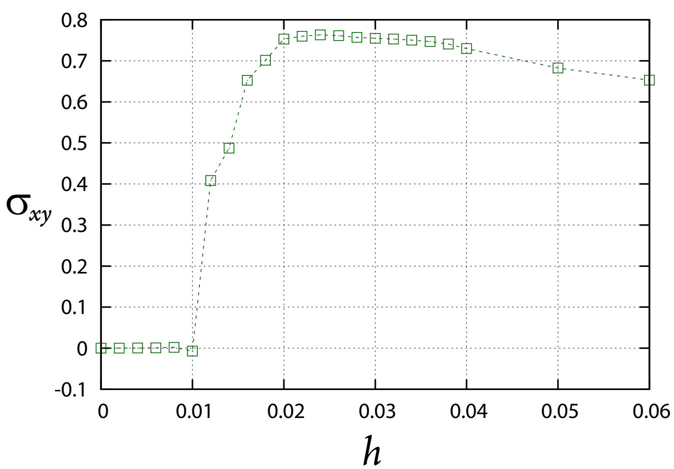

Simple model gives large Hall conductivity

(too large)

Conclusions

- The paramagnet electronic structure of $A_2Ir_2O_7$ may realize a strongly correlated analog of HgTe
- In theory, this supports a topological insulators, Weyl semimetals, and quantum criticality
- In practice, rare earth spins crucially affect low energy physics and transport.
    - Good side: makes it possible to *control* electronic state

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